



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:52 AM EDT

PDB ID : 3VMI / pdb_00003vmi
Title : Carbazole- and oxygen-bound complex between oxygenase and ferredoxin in carbazole 1,9a-dioxygenase
Authors : Ashikawa, Y.; Nojiri, H.
Deposited on : 2011-12-12
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

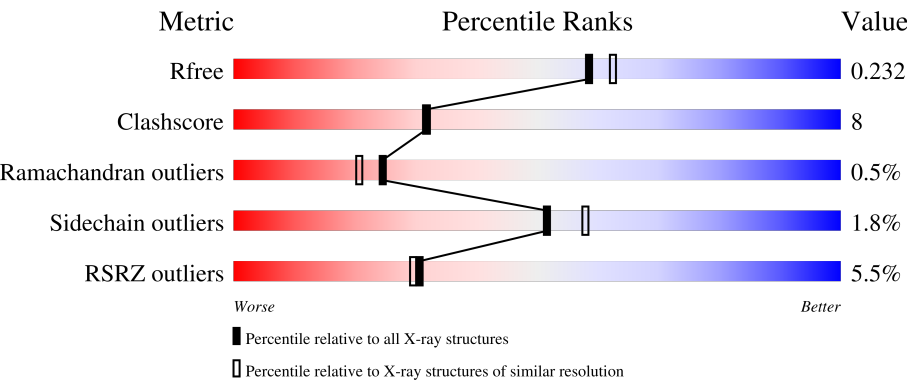
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	392	3% 83% 15% ..
1	B	392	7% 75% 22% ..
1	C	392	7% 77% 21% ..
2	D	115	6% 75% 16% 10%
2	E	115	2% 76% 17% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	115	4% 71% 18% 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12638 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Terminal oxygenase component of carbazole.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3136	2004	535	583	14			
1	B	388	Total	C	N	O	S	0	0	0
			3126	1998	532	582	14			
1	C	389	Total	C	N	O	S	0	0	0
			3136	2004	535	583	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	LEU	-	expression tag	UNP Q84II6
A	386	GLU	-	expression tag	UNP Q84II6
A	387	HIS	-	expression tag	UNP Q84II6
A	388	HIS	-	expression tag	UNP Q84II6
A	389	HIS	-	expression tag	UNP Q84II6
A	390	HIS	-	expression tag	UNP Q84II6
A	391	HIS	-	expression tag	UNP Q84II6
A	392	HIS	-	expression tag	UNP Q84II6
B	385	LEU	-	expression tag	UNP Q84II6
B	386	GLU	-	expression tag	UNP Q84II6
B	387	HIS	-	expression tag	UNP Q84II6
B	388	HIS	-	expression tag	UNP Q84II6
B	389	HIS	-	expression tag	UNP Q84II6
B	390	HIS	-	expression tag	UNP Q84II6
B	391	HIS	-	expression tag	UNP Q84II6
B	392	HIS	-	expression tag	UNP Q84II6
C	385	LEU	-	expression tag	UNP Q84II6
C	386	GLU	-	expression tag	UNP Q84II6
C	387	HIS	-	expression tag	UNP Q84II6
C	388	HIS	-	expression tag	UNP Q84II6
C	389	HIS	-	expression tag	UNP Q84II6
C	390	HIS	-	expression tag	UNP Q84II6
C	391	HIS	-	expression tag	UNP Q84II6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	392	HIS	-	expression tag	UNP Q84II6

- Molecule 2 is a protein called Ferredoxin component of carbazole.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	104	Total	C	N	O	S	0	0	0
			768	483	129	149	7			
2	E	107	Total	C	N	O	S	0	0	0
			794	499	133	155	7			
2	F	104	Total	C	N	O	S	0	0	0
			768	483	129	149	7			

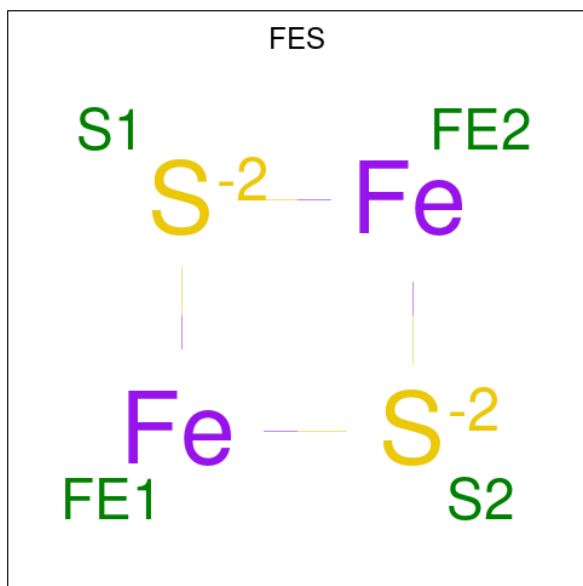
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	108	LEU	-	expression tag	UNP Q8GI16
D	109	GLU	-	expression tag	UNP Q8GI16
D	110	HIS	-	expression tag	UNP Q8GI16
D	111	HIS	-	expression tag	UNP Q8GI16
D	112	HIS	-	expression tag	UNP Q8GI16
D	113	HIS	-	expression tag	UNP Q8GI16
D	114	HIS	-	expression tag	UNP Q8GI16
D	115	HIS	-	expression tag	UNP Q8GI16
E	108	LEU	-	expression tag	UNP Q8GI16
E	109	GLU	-	expression tag	UNP Q8GI16
E	110	HIS	-	expression tag	UNP Q8GI16
E	111	HIS	-	expression tag	UNP Q8GI16
E	112	HIS	-	expression tag	UNP Q8GI16
E	113	HIS	-	expression tag	UNP Q8GI16
E	114	HIS	-	expression tag	UNP Q8GI16
E	115	HIS	-	expression tag	UNP Q8GI16
F	108	LEU	-	expression tag	UNP Q8GI16
F	109	GLU	-	expression tag	UNP Q8GI16
F	110	HIS	-	expression tag	UNP Q8GI16
F	111	HIS	-	expression tag	UNP Q8GI16
F	112	HIS	-	expression tag	UNP Q8GI16
F	113	HIS	-	expression tag	UNP Q8GI16
F	114	HIS	-	expression tag	UNP Q8GI16
F	115	HIS	-	expression tag	UNP Q8GI16

- Molecule 3 is FE (II) ION (CCD ID: FE2) (formula: Fe).

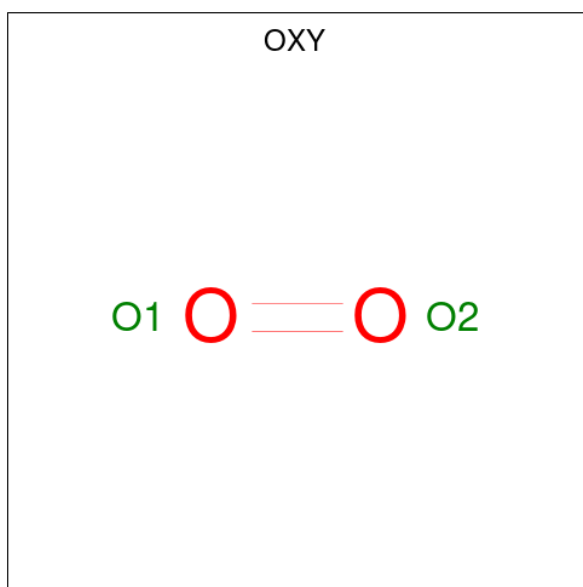
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



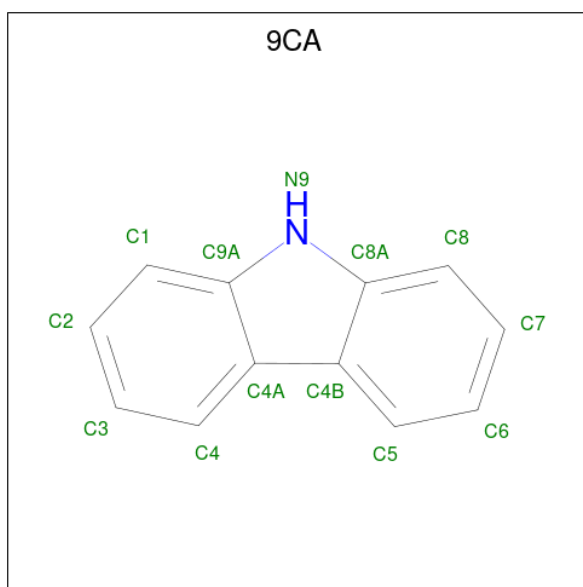
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	B	1	Total Fe S 4 2 2	0	0
4	C	1	Total Fe S 4 2 2	0	0
4	D	1	Total Fe S 4 2 2	0	0
4	E	1	Total Fe S 4 2 2	0	0
4	F	1	Total Fe S 4 2 2	0	0

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			2	2		
5	C	1	Total	O	0	0
			2	2		

- Molecule 6 is 9H-CARBAZOLE (CCD ID: 9CA) (formula: C₁₂H₉N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	N	0	0
			13	12	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	N	0	0
			13	12	1		

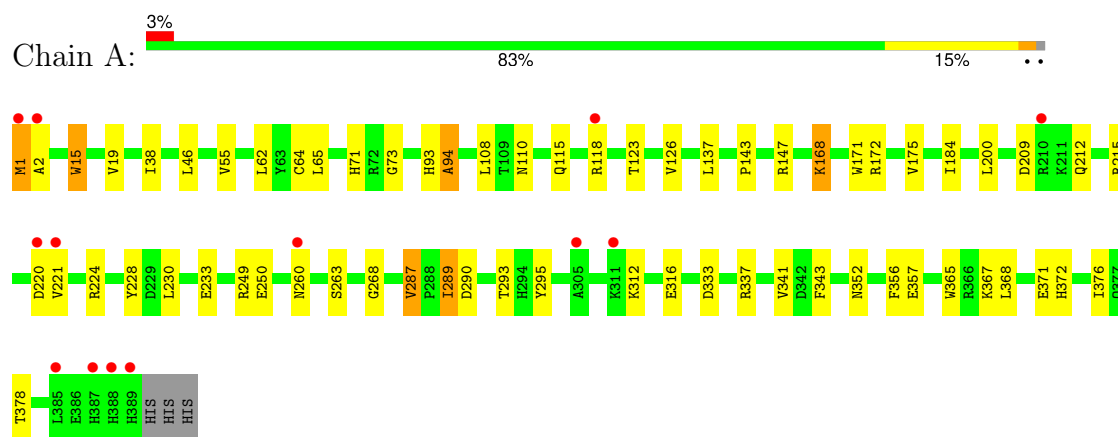
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	284	Total	O	0	0
			284	284		
7	B	237	Total	O	0	0
			237	237		
7	C	234	Total	O	0	0
			234	234		
7	D	18	Total	O	0	0
			18	18		
7	E	45	Total	O	0	0
			45	45		
7	F	33	Total	O	0	0
			33	33		

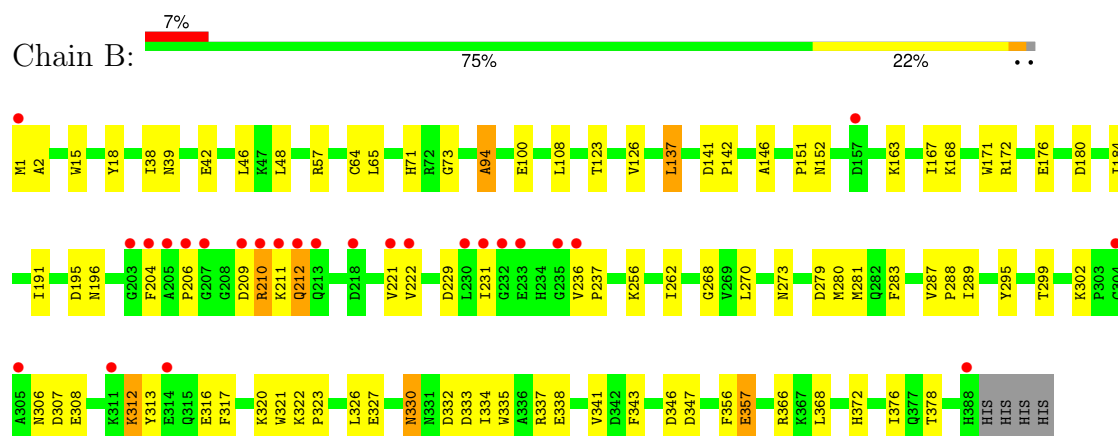
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

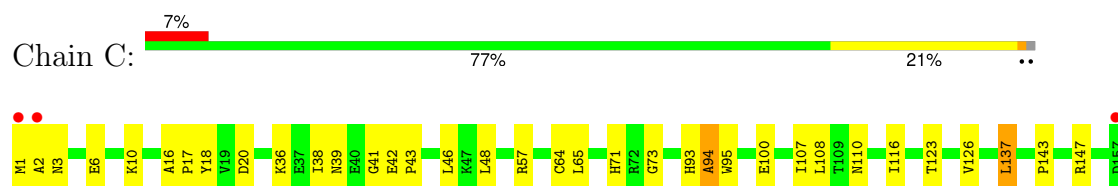
- Molecule 1: Terminal oxygenase component of carbazole

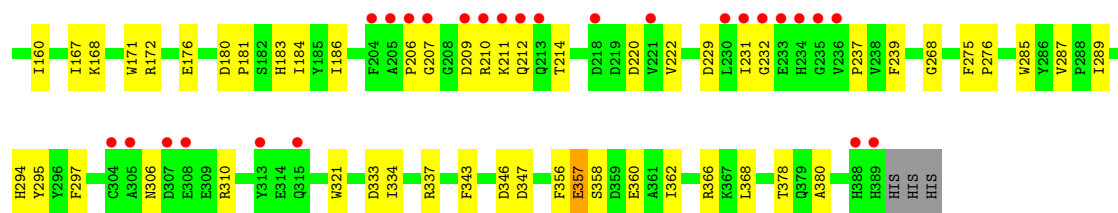


- Molecule 1: Terminal oxygenase component of carbazole

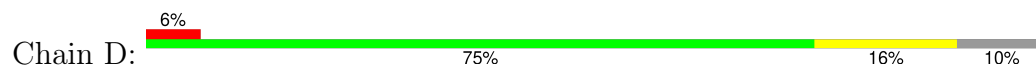


- Molecule 1: Terminal oxygenase component of carbazole

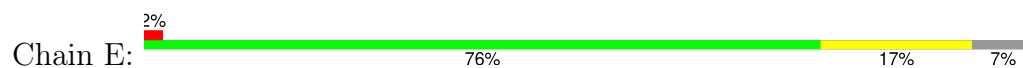




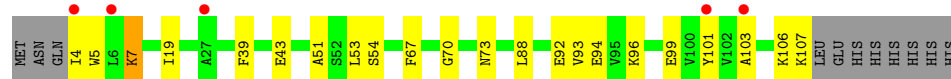
- Molecule 2: Ferredoxin component of carbazole



- Molecule 2: Ferredoxin component of carbazole



- Molecule 2: Ferredoxin component of carbazole



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.01Å 89.61Å 104.82Å 90.00° 104.18° 90.00°	Depositor
Resolution (Å)	32.68 – 2.00 32.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (32.68-2.00) 99.0 (32.68-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.240 0.199 , 0.232	Depositor DCC
R_{free} test set	5889 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12638	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, 9CA, FES, OXY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	1/3221 (0.0%)	0.89	8/4372 (0.2%)
1	B	0.43	1/3210 (0.0%)	0.91	14/4357 (0.3%)
1	C	0.38	0/3221	0.86	7/4372 (0.2%)
2	D	0.33	0/784	0.86	1/1066 (0.1%)
2	E	0.35	0/810	0.87	1/1101 (0.1%)
2	F	0.35	0/784	0.88	3/1066 (0.3%)
All	All	0.40	2/12030 (0.0%)	0.88	34/16334 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	TRP	NE1-CE2	9.98	1.48	1.37
1	B	15	TRP	NE1-CE2	9.02	1.47	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	VAL	N-CA-C	7.91	115.75	107.76
1	B	2	ALA	N-CA-C	7.69	120.63	111.02
1	B	289	ILE	N-CA-C	-6.92	105.09	111.67
1	B	141	ASP	CA-C-N	6.61	124.42	119.66
1	B	141	ASP	C-N-CA	6.61	124.42	119.66
2	F	43	GLU	N-CA-C	-6.41	101.47	110.50
1	A	357	GLU	N-CA-C	6.39	121.91	111.37
1	B	142	PRO	N-CA-C	6.26	117.28	110.58
1	C	321	TRP	N-CA-C	6.04	118.36	111.11
2	E	43	GLU	N-CA-C	-6.03	102.00	110.50
1	B	100	GLU	N-CA-C	6.00	118.78	111.82
1	B	372	HIS	N-CA-C	5.97	120.58	112.88
1	B	94	ALA	N-CA-C	5.94	119.84	112.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	GLU	N-CA-C	5.81	120.96	111.37
1	A	289	ILE	N-CA-C	-5.74	106.22	111.67
1	A	341	VAL	N-CA-C	5.74	116.38	110.36
1	A	94	ALA	N-CA-C	5.70	119.54	112.24
1	C	100	GLU	N-CA-C	5.67	117.46	111.28
1	B	341	VAL	N-CA-C	5.56	116.19	110.36
1	B	168	LYS	N-CA-C	5.49	118.11	108.56
1	A	372	HIS	N-CA-C	5.43	120.60	112.94
1	A	168	LYS	N-CA-C	5.39	117.71	109.62
1	B	221	VAL	N-CA-C	5.35	116.07	110.62
1	C	95	TRP	N-CA-C	-5.32	101.98	109.96
1	C	289	ILE	N-CA-C	-5.31	106.62	111.67
1	C	160	ILE	N-CA-C	5.29	115.58	108.17
1	A	352	ASN	N-CA-C	5.29	119.78	113.23
2	F	70	GLY	N-CA-C	-5.27	105.79	112.54
1	B	212	GLN	N-CA-C	-5.25	107.05	113.50
1	C	94	ALA	N-CA-C	5.18	118.90	112.58
2	D	86	VAL	N-CA-C	5.16	113.54	107.77
1	B	330	ASN	N-CA-C	5.13	119.39	113.18
1	C	357	GLU	N-CA-C	5.01	121.48	110.80
2	F	73	ASN	N-CA-C	-5.01	101.00	108.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3136	0	3042	39	0
1	B	3126	0	3035	61	0
1	C	3136	0	3042	52	0
2	D	768	0	745	11	0
2	E	794	0	770	13	0
2	F	768	0	745	14	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
4	A	4	0	0	1	0
4	B	4	0	0	0	0
4	C	4	0	0	1	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
6	B	13	0	9	1	0
6	C	13	0	9	1	0
7	A	284	0	0	1	0
7	B	237	0	0	2	0
7	C	234	0	0	6	0
7	D	18	0	0	0	0
7	E	45	0	0	1	0
7	F	33	0	0	3	0
All	All	12638	0	11397	187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HB3	1:A:233:GLU:HG3	1.61	0.81
1:C:210:ARG:HG3	1:C:211:LYS:H	1.45	0.79
1:C:65:LEU:HD23	1:C:123:THR:HG22	1.65	0.78
1:B:1:MET:HE3	1:B:376:ILE:H	1.49	0.77
1:A:65:LEU:HD23	1:A:123:THR:HG22	1.68	0.76
2:E:92:GLU:HB2	2:E:107:LYS:HE3	1.66	0.75
1:C:6:GLU:O	1:C:10:LYS:HG2	1.86	0.75
1:A:290:ASP:OD1	1:A:293:THR:HG22	1.85	0.75
2:F:4:ILE:HG13	2:F:5:TRP:H	1.53	0.73
1:B:209:ASP:OD2	1:B:212:GLN:HB2	1.89	0.73
1:B:322:LYS:HB3	1:B:323:PRO:HD3	1.73	0.70
2:D:7:LYS:HG2	2:D:101:TYR:CE1	2.26	0.70
2:E:108:LEU:O	2:E:109:GLU:HB3	1.91	0.69
1:A:1:MET:HB2	1:A:378:THR:HG21	1.73	0.69
1:B:38:ILE:HG23	1:B:57:ARG:HH21	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:HB	1:A:293:THR:HG23	1.74	0.68
1:C:220:ASP:OD1	1:C:222:VAL:HG22	1.98	0.64
1:B:210:ARG:HG3	7:B:817:HOH:O	1.97	0.63
1:C:1:MET:HB2	1:C:378:THR:HG21	1.81	0.61
1:B:206:PRO:HG3	1:B:357:GLU:HB3	1.82	0.61
1:B:210:ARG:HD3	1:B:211:LYS:HG3	1.81	0.61
2:F:53:LEU:CD1	2:F:88:LEU:HD11	2.30	0.61
1:C:2:ALA:HA	7:C:818:HOH:O	2.00	0.60
2:D:6:LEU:HD23	2:D:7:LYS:N	2.17	0.59
1:C:206:PRO:HG2	1:C:357:GLU:HB3	1.84	0.59
2:D:51:ALA:HB2	2:D:67:PHE:CG	2.39	0.58
1:B:210:ARG:HH11	1:B:211:LYS:NZ	2.01	0.58
2:E:108:LEU:O	2:E:109:GLU:CB	2.51	0.58
2:E:4:ILE:HG23	2:E:5:TRP:CD1	2.39	0.58
1:C:94:ALA:HB1	1:C:108:LEU:HB2	1.85	0.58
1:C:48:LEU:HD23	1:C:137:LEU:HD23	1.85	0.57
1:B:163:LYS:HD3	7:B:546:HOH:O	2.04	0.57
1:B:1:MET:HB3	1:B:378:THR:HG21	1.85	0.57
1:A:312:LYS:HE2	1:A:316:GLU:OE2	2.03	0.57
1:C:38:ILE:HG23	1:C:57:ARG:HH21	1.69	0.56
1:C:287:VAL:HB	1:C:295:TYR:HB2	1.87	0.56
1:A:94:ALA:HB1	1:A:108:LEU:HB2	1.88	0.56
1:C:360:GLU:HG3	7:C:525:HOH:O	2.04	0.56
2:F:4:ILE:HG13	2:F:5:TRP:N	2.20	0.56
1:B:287:VAL:HB	1:B:295:TYR:HB2	1.87	0.56
1:B:191:ILE:O	1:B:195:ASP:HB2	2.06	0.56
1:B:38:ILE:HG23	1:B:57:ARG:NH2	2.22	0.55
2:F:19:ILE:HG21	2:F:54:SER:HA	1.89	0.55
1:C:39:ASN:HB2	1:C:42:GLU:OE2	2.07	0.55
1:B:1:MET:CE	1:B:376:ILE:H	2.17	0.55
1:B:204:PHE:CD2	1:B:231:ILE:HD12	2.41	0.55
1:B:333:ASP:O	1:B:337:ARG:HG3	2.06	0.55
1:A:220:ASP:HB2	1:A:224:ARG:HB2	1.89	0.54
1:A:287:VAL:HB	1:A:295:TYR:HB2	1.89	0.54
2:F:96:LYS:HE2	2:F:101:TYR:CZ	2.43	0.54
1:B:94:ALA:HB1	1:B:108:LEU:HB2	1.90	0.54
1:C:306:ASN:O	1:C:310:ARG:HG3	2.08	0.54
1:B:167:ILE:HD12	1:B:334:ILE:HG23	1.89	0.53
1:C:181:PRO:HG2	1:C:358:SER:HB2	1.89	0.53
1:C:176:GLU:O	1:C:180:ASP:HB2	2.07	0.53
1:A:290:ASP:CG	1:A:293:THR:HG22	2.33	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:HD23	1:B:137:LEU:HD23	1.91	0.53
1:B:39:ASN:HB2	1:B:42:GLU:OE1	2.09	0.53
1:C:210:ARG:HA	7:C:615:HOH:O	2.09	0.52
1:A:228:TYR:CD1	1:A:263:SER:HB3	2.44	0.52
2:D:7:LYS:HG2	2:D:101:TYR:HE1	1.73	0.52
1:B:334:ILE:O	1:B:338:GLU:HG3	2.09	0.52
1:A:184:ILE:HD11	1:A:200:LEU:CD1	2.40	0.52
1:C:210:ARG:HG3	1:C:211:LYS:N	2.21	0.52
2:E:5:TRP:CZ3	2:E:94:GLU:HG2	2.45	0.52
1:A:1:MET:O	1:A:2:ALA:HB3	2.10	0.52
1:A:143:PRO:HG3	1:A:147:ARG:CZ	2.40	0.52
1:B:176:GLU:O	1:B:180:ASP:HB2	2.11	0.51
1:B:262:ILE:CG2	1:B:270:LEU:HD11	2.40	0.51
1:B:262:ILE:HG22	1:B:270:LEU:HD11	1.92	0.51
1:C:107:ILE:HG13	1:C:116:ILE:HG12	1.92	0.51
2:D:19:ILE:HG21	2:D:54:SER:HA	1.94	0.51
1:A:168:LYS:HE2	7:A:784:HOH:O	2.11	0.50
1:C:183:HIS:O	1:C:186:ILE:HG12	2.11	0.50
2:F:99:GLU:HB3	2:F:101:TYR:HE1	1.77	0.50
1:C:171:TRP:CE2	1:C:172:ARG:HG3	2.46	0.50
1:C:285:TRP:HB2	1:C:297:PHE:HB3	1.94	0.50
2:F:106:LYS:O	2:F:107:LYS:HB2	2.11	0.50
1:B:312:LYS:O	1:B:316:GLU:HG3	2.12	0.50
1:A:171:TRP:CE2	1:A:172:ARG:HG3	2.47	0.50
1:B:94:ALA:CB	1:B:108:LEU:HB2	2.42	0.50
1:B:280:MET:HE3	1:B:313:TYR:CE1	2.47	0.50
1:B:210:ARG:C	1:B:212:GLN:H	2.20	0.49
1:B:210:ARG:HD2	1:B:211:LYS:HZ3	1.77	0.49
1:B:229:ASP:OD2	1:B:231:ILE:HG23	2.13	0.49
1:C:39:ASN:HB2	1:C:42:GLU:CD	2.37	0.49
1:C:38:ILE:HG23	1:C:57:ARG:NH2	2.28	0.49
2:D:90:VAL:HG23	2:D:107:LYS:HG2	1.94	0.49
2:F:39:PHE:O	2:F:93:VAL:HG11	2.13	0.49
2:F:92:GLU:HG2	2:F:103:ALA:HB2	1.95	0.49
2:D:92:GLU:HG2	2:D:107:LYS:HE2	1.95	0.49
2:E:10:ALA:HB3	2:E:13:ASP:OD2	2.13	0.48
1:A:93:HIS:HB2	4:A:401:FES:S1	2.53	0.48
1:B:171:TRP:CE2	1:B:172:ARG:HG3	2.48	0.48
1:B:283:PHE:HB2	1:B:299:THR:OG1	2.13	0.48
1:A:1:MET:H1	1:A:376:ILE:HG21	1.79	0.48
1:A:1:MET:HB2	1:A:378:THR:CG2	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:HB2	1:A:230:LEU:HD11	1.94	0.48
1:C:168:LYS:HE2	7:C:605:HOH:O	2.14	0.48
1:A:15:TRP:HD1	1:A:19:VAL:HG23	1.79	0.47
1:A:73:GLY:HA3	1:C:343:PHE:CG	2.49	0.47
1:A:333:ASP:O	1:A:337:ARG:HG3	2.15	0.47
2:E:51:ALA:HB2	2:E:67:PHE:CG	2.48	0.47
1:A:367:LYS:O	1:A:371:GLU:HG3	2.14	0.47
1:B:326:LEU:O	1:B:330:ASN:HB2	2.15	0.47
2:E:19:ILE:HD11	2:E:58:LEU:HB2	1.97	0.47
1:A:38:ILE:CD1	1:A:55:VAL:HG12	2.45	0.47
2:F:51:ALA:HB2	2:F:67:PHE:CG	2.49	0.47
1:A:94:ALA:CB	1:A:108:LEU:HB2	2.45	0.47
1:B:222:VAL:O	1:B:222:VAL:HG12	2.14	0.47
1:B:210:ARG:HH11	1:B:211:LYS:HZ3	1.60	0.46
1:C:93:HIS:HB2	4:C:401:FES:S1	2.56	0.46
1:A:118:ARG:HG3	7:F:116:HOH:O	2.15	0.46
1:B:280:MET:HE3	1:B:313:TYR:HE1	1.80	0.46
2:D:95:VAL:HG22	2:D:100:VAL:HG22	1.97	0.46
1:C:333:ASP:O	1:C:337:ARG:HG3	2.16	0.46
1:C:110:ASN:C	1:C:110:ASN:HD22	2.24	0.46
1:C:143:PRO:HG3	1:C:147:ARG:CZ	2.46	0.46
1:C:176:GLU:HG2	1:C:362:ILE:HG23	1.96	0.46
1:A:249:ARG:HG3	1:A:250:GLU:N	2.31	0.46
2:F:93:VAL:HG23	2:F:101:TYR:O	2.16	0.46
1:A:1:MET:N	1:A:376:ILE:HG21	2.31	0.46
1:A:175:VAL:HG11	1:A:365:TRP:CE2	2.52	0.45
1:B:343:PHE:CG	1:C:73:GLY:HA3	2.52	0.45
1:C:167:ILE:HB	1:C:294:HIS:CE1	2.52	0.45
1:B:332:ASP:HA	1:B:335:TRP:NE1	2.32	0.45
1:C:231:ILE:HG13	1:C:232:GLY:N	2.31	0.45
1:C:3:ASN:HB2	1:C:20:ASP:OD1	2.17	0.45
1:C:209:ASP:CG	1:C:212:GLN:HE21	2.25	0.45
1:A:38:ILE:HD13	1:A:62:LEU:HD22	1.98	0.44
1:C:346:ASP:O	1:C:347:ASP:HB2	2.17	0.44
2:D:14:MET:HE3	2:D:20:ARG:HB2	1.98	0.44
1:C:94:ALA:CB	1:C:108:LEU:HB2	2.48	0.44
2:E:4:ILE:HG23	2:E:5:TRP:N	2.32	0.44
1:B:306:ASN:OD1	1:B:308:GLU:HB2	2.18	0.44
1:A:220:ASP:OD1	1:A:221:VAL:N	2.49	0.44
1:B:65:LEU:HD23	1:B:123:THR:HG22	2.00	0.43
1:C:210:ARG:C	1:C:212:GLN:N	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:PRO:HG3	1:B:357:GLU:CB	2.48	0.43
1:B:236:VAL:HA	1:B:237:PRO:HD3	1.86	0.43
1:C:64:CYS:HB2	1:C:126:VAL:HG21	2.00	0.43
2:E:92:GLU:OE1	2:E:107:LYS:NZ	2.51	0.43
1:B:1:MET:HB3	1:B:378:THR:CG2	2.48	0.43
1:B:196:ASN:O	1:B:256:LYS:HD2	2.19	0.43
1:A:175:VAL:HG11	1:A:365:TRP:CZ2	2.54	0.43
1:B:273:ASN:OD1	1:B:281:MET:HG2	2.18	0.43
1:C:36:LYS:NZ	7:C:466:HOH:O	2.51	0.43
1:A:65:LEU:CD2	1:A:123:THR:HG22	2.45	0.43
2:E:86:VAL:HA	2:E:87:PRO:HD3	1.89	0.43
1:C:275:PHE:CG	1:C:276:PRO:HA	2.54	0.43
1:C:18:TYR:CE2	1:C:366:ARG:HG2	2.54	0.42
1:B:287:VAL:HA	1:B:288:PRO:HD3	1.91	0.42
1:B:346:ASP:O	1:B:347:ASP:HB2	2.20	0.42
1:C:237:PRO:HB2	1:C:239:PHE:CE2	2.55	0.42
2:F:5:TRP:CH2	2:F:94:GLU:HG3	2.55	0.42
1:B:210:ARG:C	1:B:212:GLN:N	2.78	0.42
1:B:322:LYS:O	1:B:327:GLU:HG3	2.20	0.42
1:A:64:CYS:HB2	1:A:126:VAL:CG2	2.50	0.42
1:B:279:ASP:OD2	1:B:302:LYS:NZ	2.51	0.42
2:F:7:LYS:HE3	7:F:806:HOH:O	2.20	0.42
1:C:184:ILE:HG21	6:C:2002:9CA:C6	2.50	0.42
1:A:343:PHE:CG	1:B:73:GLY:HA3	2.55	0.41
1:B:302:LYS:HD3	1:B:313:TYR:CD1	2.55	0.41
1:B:210:ARG:CD	1:B:211:LYS:HZ3	2.32	0.41
1:B:18:TYR:CE2	1:B:366:ARG:HG2	2.55	0.41
1:B:151:PRO:O	1:B:152:ASN:HB2	2.21	0.41
1:B:320:LYS:C	1:B:323:PRO:HD2	2.45	0.41
1:A:115:GLN:HA	1:A:115:GLN:OE1	2.20	0.41
2:D:10:ALA:HB3	2:D:13:ASP:OD2	2.21	0.41
1:B:184:ILE:HG21	6:B:2001:9CA:C6	2.50	0.41
1:C:380:ALA:HB3	7:C:486:HOH:O	2.20	0.41
1:C:229:ASP:OD1	1:C:231:ILE:HG23	2.21	0.41
1:A:209:ASP:OD1	1:A:212:GLN:HG3	2.21	0.41
1:B:210:ARG:HH11	1:B:211:LYS:HG3	1.86	0.41
1:A:110:ASN:C	1:A:110:ASN:HD22	2.28	0.41
1:C:16:ALA:N	1:C:17:PRO:CD	2.84	0.41
2:E:20:ARG:HD3	7:E:850:HOH:O	2.21	0.41
1:C:38:ILE:HG23	1:C:38:ILE:O	2.20	0.41
1:C:41:GLY:O	1:C:43:PRO:HD3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:PHE:HA	1:B:321:TRP:HB2	2.02	0.40
2:F:106:LYS:NZ	7:F:591:HOH:O	2.49	0.40
1:B:64:CYS:HB2	1:B:126:VAL:CG2	2.51	0.40
1:B:146:ALA:HB3	1:B:222:VAL:HG11	2.02	0.40
1:C:167:ILE:HD12	1:C:334:ILE:HG23	2.02	0.40
1:C:231:ILE:HG13	1:C:232:GLY:H	1.86	0.40
2:D:90:VAL:HG23	2:D:107:LYS:CG	2.51	0.40
2:E:19:ILE:HG21	2:E:54:SER:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/392 (99%)	369 (95%)	16 (4%)	2 (0%)	24	21
1	B	386/392 (98%)	354 (92%)	30 (8%)	2 (0%)	24	21
1	C	387/392 (99%)	362 (94%)	22 (6%)	3 (1%)	16	11
2	D	102/115 (89%)	94 (92%)	8 (8%)	0	100	100
2	E	105/115 (91%)	100 (95%)	5 (5%)	0	100	100
2	F	102/115 (89%)	100 (98%)	2 (2%)	0	100	100
All	All	1469/1521 (97%)	1379 (94%)	83 (6%)	7 (0%)	24	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	GLY
1	A	268	GLY
1	C	268	GLY
1	A	71	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	71	HIS
1	B	71	HIS
1	C	207	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/339 (99%)	330 (98%)	6 (2%)	51	58
1	B	335/339 (99%)	328 (98%)	7 (2%)	47	52
1	C	336/339 (99%)	331 (98%)	5 (2%)	57	64
2	D	82/93 (88%)	81 (99%)	1 (1%)	63	70
2	E	85/93 (91%)	83 (98%)	2 (2%)	43	47
2	F	82/93 (88%)	81 (99%)	1 (1%)	63	70
All	All	1256/1296 (97%)	1234 (98%)	22 (2%)	51	58

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	46	LEU
1	A	137	LEU
1	A	260	ASN
1	A	356	PHE
1	A	368	LEU
1	B	46	LEU
1	B	137	LEU
1	B	210	ARG
1	B	307	ASP
1	B	312	LYS
1	B	356	PHE
1	B	368	LEU
1	C	46	LEU
1	C	137	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	214	THR
1	C	356	PHE
1	C	368	LEU
2	D	105	GLU
2	E	6	LEU
2	E	96	LYS
2	F	7	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	213	GLN
1	A	234	HIS
1	A	372	HIS
1	A	389	HIS
1	B	52	ASN
1	B	110	ASN
1	B	127	GLN
1	B	212	GLN
1	B	234	HIS
1	B	292	ASN
1	B	315	GLN
1	C	110	ASN
1	C	127	GLN
1	C	177	ASN
1	C	212	GLN
1	C	234	HIS
1	C	315	GLN
1	C	379	GLN
1	C	388	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	OXY	A	601	3	1,1,1	0.99	0	-		
6	9CA	B	2001	-	15,15,15	1.36	3 (20%)	21,21,21	1.00	0
5	OXY	C	603	3	1,1,1	0.99	0	-		
4	FES	B	401	1	0,4,4	-	-	-		
4	FES	D	201	2	0,4,4	-	-	-		
4	FES	E	201	2	0,4,4	-	-	-		
4	FES	F	201	2	0,4,4	-	-	-		
4	FES	A	401	1	0,4,4	-	-	-		
5	OXY	B	602	3	1,1,1	1.01	0	-		
4	FES	C	401	1	0,4,4	-	-	-		
6	9CA	C	2002	-	15,15,15	1.37	3 (20%)	21,21,21	0.97	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	9CA	B	2001	-	-	-	0/3/3/3
4	FES	B	401	1	-	-	0/1/1/1
4	FES	D	201	2	-	-	0/1/1/1
4	FES	E	201	2	-	-	0/1/1/1
4	FES	F	201	2	-	-	0/1/1/1
4	FES	A	401	1	-	-	0/1/1/1
4	FES	C	401	1	-	-	0/1/1/1
6	9CA	C	2002	-	-	-	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2002	9CA	C4B-C4A	-2.84	1.39	1.46
6	B	2001	9CA	C4B-C4A	-2.80	1.39	1.46
6	C	2002	9CA	C9A-N9	-2.78	1.33	1.38
6	B	2001	9CA	C9A-N9	-2.78	1.33	1.38
6	C	2002	9CA	C8A-N9	-2.77	1.33	1.38
6	B	2001	9CA	C8A-N9	-2.76	1.33	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	2001	9CA	1	0
4	A	401	FES	1	0
4	C	401	FES	1	0
6	C	2002	9CA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	389/392 (99%)	0.08	13 (3%)	49	48	25, 36, 49, 59	0
1	B	388/392 (98%)	0.41	26 (6%)	24	22	27, 39, 54, 59	0
1	C	389/392 (99%)	0.43	29 (7%)	20	19	29, 39, 52, 62	0
2	D	104/115 (90%)	0.76	7 (6%)	24	22	33, 48, 56, 58	0
2	E	107/115 (93%)	0.45	2 (1%)	66	66	31, 42, 51, 57	0
2	F	104/115 (90%)	0.82	5 (4%)	35	34	35, 46, 53, 58	0
All	All	1481/1521 (97%)	0.39	82 (5%)	30	29	25, 39, 53, 62	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	7.1
1	A	1	MET	7.0
1	B	204	PHE	6.5
1	B	1	MET	6.5
1	B	205	ALA	6.2
1	C	205	ALA	5.7
1	C	204	PHE	5.5
1	C	230	LEU	5.3
1	C	209	ASP	5.2
1	C	236	VAL	5.2
1	B	206	PRO	4.7
1	B	230	LEU	4.6
1	B	212	GLN	4.6
1	B	236	VAL	4.5
1	B	209	ASP	4.2
1	C	235	GLY	4.2
1	B	231	ILE	4.1
1	A	389	HIS	4.0
1	C	206	PRO	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	213	GLN	3.8
1	C	213	GLN	3.6
2	F	4	ILE	3.6
1	C	2	ALA	3.6
1	C	305	ALA	3.6
1	B	210	ARG	3.4
1	B	221	VAL	3.4
2	D	4	ILE	3.3
1	C	233	GLU	3.3
1	C	389	HIS	3.1
1	C	315	GLN	3.1
1	A	387	HIS	3.1
1	B	235	GLY	3.0
1	C	232	GLY	3.0
1	A	221	VAL	3.0
2	F	101	TYR	3.0
2	F	103	ALA	2.9
1	B	222	VAL	2.9
1	C	212	GLN	2.9
1	C	313	TYR	2.9
1	B	305	ALA	2.9
1	C	307	ASP	2.8
2	E	98	GLY	2.9
1	A	220	ASP	2.8
1	B	314	GLU	2.8
1	C	231	ILE	2.8
1	C	211	LYS	2.8
2	D	37	ASP	2.7
1	A	2	ALA	2.7
1	B	388	HIS	2.7
1	B	203	GLY	2.6
1	B	211	LYS	2.6
1	C	157	ASP	2.6
1	C	207	GLY	2.5
1	C	210	ARG	2.5
2	E	37	ASP	2.5
1	B	207	GLY	2.4
2	D	5	TRP	2.4
1	A	385	LEU	2.3
1	B	232	GLY	2.3
2	D	99	GLU	2.3
1	A	118	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	233	GLU	2.3
1	C	218	ASP	2.3
1	C	234	HIS	2.3
1	A	210	ARG	2.3
1	A	388	HIS	2.2
1	C	221	VAL	2.2
2	D	95	VAL	2.2
2	F	6	LEU	2.2
1	B	218	ASP	2.1
1	C	304	CYS	2.1
1	A	260	ASN	2.1
1	B	157	ASP	2.1
1	C	388	HIS	2.1
2	F	27	ALA	2.1
1	A	311	LYS	2.1
1	B	304	CYS	2.0
1	B	311	LYS	2.0
2	D	7	LYS	2.0
1	C	308	GLU	2.0
1	A	305	ALA	2.0
2	D	98	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	9CA	C	2002	13/13	0.71	0.16	44,47,48,48	0
6	9CA	B	2001	13/13	0.82	0.12	47,48,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	OXY	B	602	2/2	0.92	0.10	57,57,57,57	0
5	OXY	A	601	2/2	0.96	0.11	43,43,43,45	0
5	OXY	C	603	2/2	0.96	0.10	49,49,49,51	0
4	FES	C	401	4/4	0.98	0.04	35,35,36,37	0
4	FES	F	201	4/4	0.99	0.07	31,34,35,36	0
4	FES	A	401	4/4	0.99	0.04	30,31,32,33	0
4	FES	B	401	4/4	0.99	0.05	24,29,29,30	0
3	FE2	B	501	1/1	0.99	0.04	44,44,44,44	0
4	FES	D	201	4/4	0.99	0.03	33,33,33,33	0
4	FES	E	201	4/4	0.99	0.04	32,33,33,33	0
3	FE2	C	501	1/1	1.00	0.06	35,35,35,35	0
3	FE2	A	501	1/1	1.00	0.03	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.