Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2026 – 09:55 pm BST

PDB ID	:	5HL4 / pdb_00005hl4
Title	:	Acoustic injectors for drop-on-demand serial femtosecond crystallography
Authors	:	Roessler, C.G.; Agarwal, R.; Allaire, M.; Alonso-Mori, R.; Andi, B.; Bachega, J.F.R.; Bommer, M.; Brewster, A.S.; Browne, M.C.; Chatterjee, R.; Cho, E.; Cohen, A.E.; Cowan, M.; Datwani, S.; Davidson, V.L.; Defever, J.; Eaton, B.; Ellson, R.; Feng, Y.; Ghislain, L.P.; Glownia, J.M.; Han, G.; Hattne, J.; Hellmich, J.; Heroux, A.; Ibrahim, M.; Kern, J.; Kuczewski, A.; Lemke, H.T.; Liu, P.; Majlof, L.; McClintock, W.M.; Myers, S.; Nelsen, S.; Olechno, J.; Orville, A.M.; Sauter, N.K.; Soares, A.S.; Soltis, M.S.; Song, H.; Stearns, R.G.; Tran, R.; Tsai, Y.; Uervirojnangkoorn, M.; Wilmot, C.M.; Yachandra, V.; Yano, J.; Yukl, E.T.; Zhu, D.; Zouni, A.
Deposited on	:	2016-01-14
Resolution	:	2.20 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 (i) 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 (1)) were used in the production of this report:

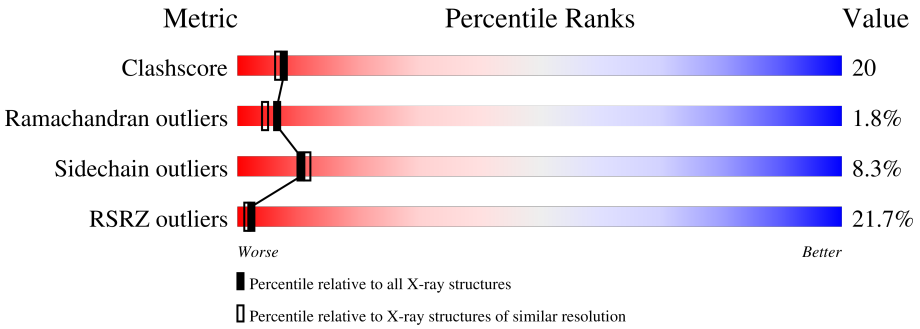
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0

1 Overall quality at a glance

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

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 <=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	412	21% 60% 29% 7% .

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

2 Entry composition

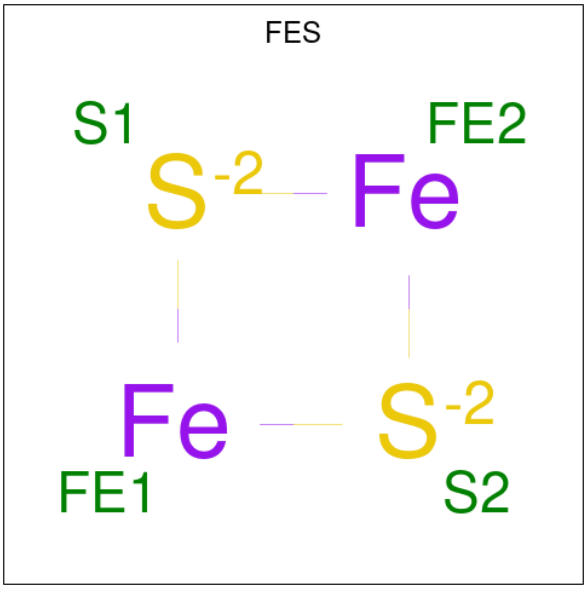
There are 5 unique types of molecules in this entry. The entry contains 3305 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ring-hydroxylating dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	397	3159	2014	549	581	15	0	0	0

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

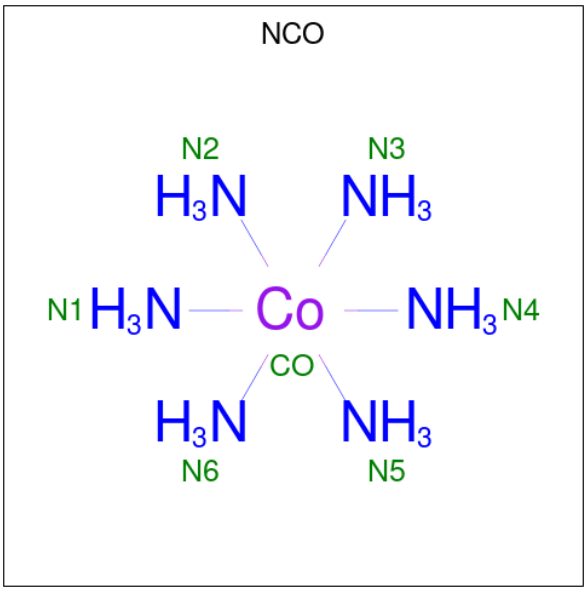


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	4	2	2	0	0

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

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

- Molecule 4 is COBALT HEXAMMINE(III) (CCD ID: NCO) (formula: $CoH_{18}N_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Co	N	0	0
			7	1	6		

- Molecule 5 is water.

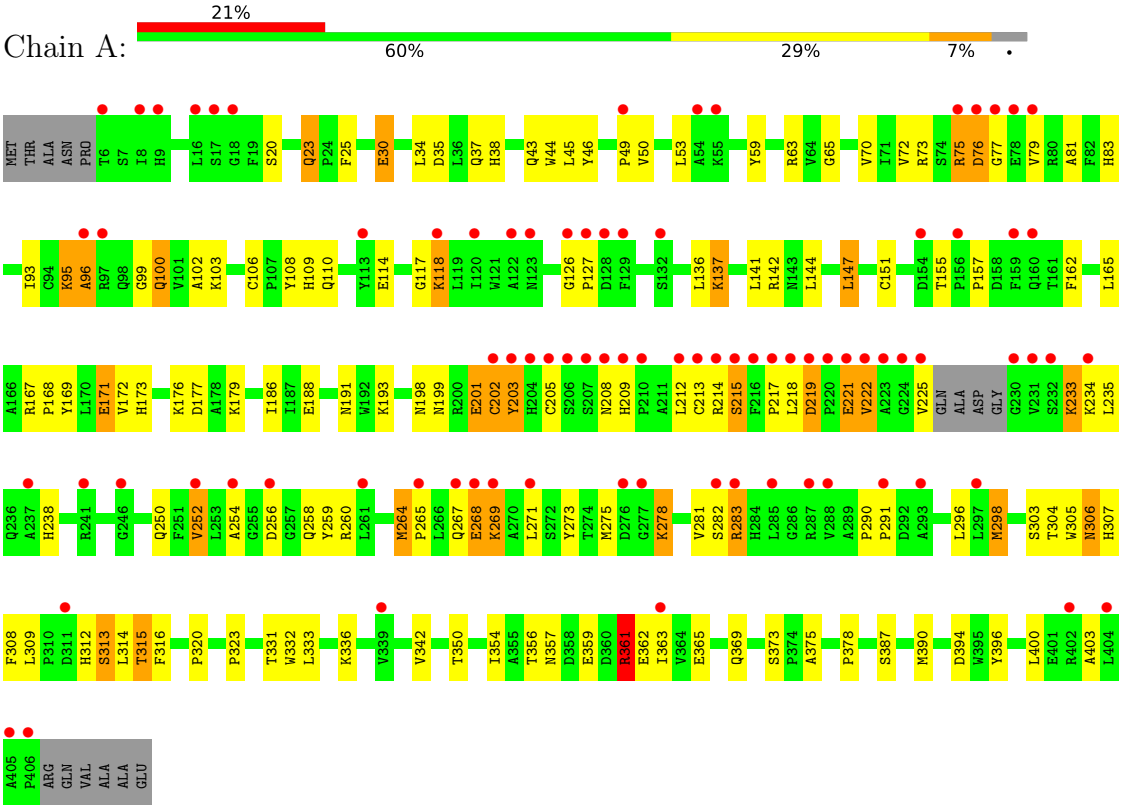
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	134	Total	O	0	0
			134	134		

3 Residue-property plots (i)

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: Ring-hydroxylating dioxygenase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.43Å 98.43Å 180.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	90.04 – 2.20 90.04 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (90.04-2.20) 99.6 (90.04-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.269 , 0.330 0.308 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	22.1	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 24.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	3305	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, FE, NCO

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	0.89	1/3247 (0.0%)	1.11	12/4421 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	PRO	N-CA	-5.16	1.41	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	126	GLY	CA-C-N	8.35	127.65	118.97
1	A	126	GLY	C-N-CA	8.35	127.65	118.97
1	A	23	GLN	CA-C-N	-8.26	111.22	119.56
1	A	23	GLN	C-N-CA	-8.26	111.22	119.56
1	A	315	THR	CB-CA-C	-6.93	97.65	109.51
1	A	199	ASN	N-CA-C	6.25	118.09	111.28
1	A	354	ILE	N-CA-C	-6.00	104.66	110.72
1	A	114	GLU	N-CA-C	-5.66	103.18	110.19
1	A	304	THR	N-CA-C	5.46	117.69	109.23
1	A	361	ARG	N-CA-C	-5.43	105.05	110.97
1	A	357	ASN	N-CA-C	5.34	117.10	111.28
1	A	264	MET	N-CA-C	5.03	117.25	110.31

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	GLU	Peptide
1	A	202	CYS	Peptide

5.2 Too-close contacts (i)

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	3159	0	3059	125	0
2	A	4	0	0	1	0
3	A	1	0	0	0	0
4	A	7	0	0	0	0
5	A	134	0	0	36	0
All	All	3305	0	3059	125	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 20.

All (125) 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:217:PRO:HB2	1:A:222:VAL:HG21	1.48	0.94
1:A:108:TYR:HB2	5:A:632:HOH:O	1.75	0.86
1:A:53:LEU:O	1:A:73:ARG:NH2	2.11	0.83
1:A:314:LEU:HG	5:A:627:HOH:O	1.78	0.82
1:A:141:LEU:HB2	5:A:628:HOH:O	1.80	0.80
1:A:46:TYR:OH	1:A:315:THR:HG21	1.81	0.79
1:A:217:PRO:CB	1:A:222:VAL:HG21	2.12	0.79
1:A:314:LEU:HB2	5:A:605:HOH:O	1.82	0.79
1:A:37:GLN:HG2	1:A:38:HIS:CE1	2.24	0.72
1:A:106:CYS:SG	5:A:632:HOH:O	2.46	0.72
1:A:102:ALA:HB1	5:A:717:HOH:O	1.90	0.71
1:A:387:SER:HA	1:A:390:MET:HE3	1.73	0.70
1:A:268:GLU:O	1:A:269:LYS:HB2	1.92	0.69
1:A:234:LYS:HB2	5:A:606:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLU:OE2	1:A:203:TYR:HB3	1.95	0.66
1:A:222:VAL:HA	1:A:264:MET:HE2	1.76	0.65
1:A:169:TYR:OH	1:A:250:GLN:O	2.13	0.65
1:A:127:PRO:HA	5:A:706:HOH:O	1.97	0.64
1:A:25:PHE:O	1:A:193:LYS:CE	2.46	0.64
1:A:59:TYR:HB2	1:A:72:VAL:HG12	1.79	0.64
1:A:332:TRP:CE2	1:A:350:THR:HG22	2.33	0.64
1:A:59:TYR:CB	1:A:72:VAL:HG12	2.27	0.64
1:A:235:LEU:HD11	1:A:264:MET:HE1	1.79	0.63
1:A:95:LYS:O	1:A:96:ALA:O	2.16	0.63
1:A:234:LYS:CB	5:A:606:HOH:O	2.47	0.62
1:A:283:ARG:HG2	1:A:283:ARG:HH11	1.64	0.62
1:A:217:PRO:HG2	1:A:222:VAL:HG11	1.82	0.62
1:A:83:HIS:HD2	1:A:137:LYS:HB3	1.65	0.61
1:A:214:ARG:HG2	5:A:639:HOH:O	1.99	0.61
1:A:171:GLU:HB3	5:A:710:HOH:O	2.01	0.61
1:A:250:GLN:HG3	5:A:686:HOH:O	2.00	0.61
1:A:35:ASP:OD2	1:A:193:LYS:NZ	2.34	0.60
1:A:50:VAL:O	1:A:50:VAL:HG22	2.02	0.59
1:A:307:HIS:N	5:A:605:HOH:O	2.34	0.59
1:A:63:ARG:CZ	1:A:65:GLY:O	2.50	0.59
1:A:95:LYS:O	1:A:96:ALA:C	2.46	0.58
1:A:298:MET:HG2	5:A:652:HOH:O	2.03	0.58
1:A:208:ASN:CG	1:A:363:ILE:HD11	2.29	0.57
1:A:155:THR:O	1:A:155:THR:OG1	2.15	0.57
1:A:283:ARG:HH11	1:A:283:ARG:CG	2.17	0.57
1:A:225:VAL:HA	5:A:694:HOH:O	2.04	0.56
1:A:93:ILE:HD11	1:A:136:LEU:HD21	1.87	0.56
1:A:198:ASN:O	1:A:201:GLU:HG2	2.06	0.56
1:A:109:HIS:HB2	2:A:501:FES:S1	2.46	0.55
1:A:109:HIS:C	1:A:110:GLN:OE1	2.49	0.55
1:A:162:PHE:HB2	1:A:259:TYR:CE2	2.41	0.55
1:A:188:GLU:HG2	1:A:361:ARG:HB2	1.89	0.54
1:A:81:ALA:HB3	5:A:628:HOH:O	2.09	0.53
1:A:110:GLN:OE1	1:A:110:GLN:N	2.42	0.52
1:A:20:SER:O	1:A:378:PRO:HB3	2.09	0.52
1:A:306:ASN:HB2	1:A:308:PHE:CE1	2.44	0.52
1:A:332:TRP:CD1	5:A:627:HOH:O	2.63	0.52
1:A:99:GLY:C	1:A:100:GLN:HG2	2.34	0.51
1:A:219:ASP:O	1:A:222:VAL:HG23	2.10	0.51
1:A:25:PHE:O	1:A:193:LYS:HE3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ASP:HB3	5:A:647:HOH:O	2.11	0.51
1:A:208:ASN:CB	1:A:363:ILE:HD11	2.41	0.51
1:A:309:LEU:HD12	1:A:312:HIS:CE1	2.45	0.50
1:A:323:PRO:HD2	5:A:718:HOH:O	2.10	0.50
1:A:167:ARG:HB3	1:A:168:PRO:HD3	1.93	0.50
1:A:44:TRP:CE3	1:A:151:CYS:HB2	2.47	0.50
1:A:103:LYS:HE2	5:A:717:HOH:O	2.10	0.50
1:A:273:TYR:OH	1:A:307:HIS:ND1	2.42	0.50
1:A:70:VAL:HG22	1:A:72:VAL:HG13	1.94	0.49
1:A:235:LEU:HD11	1:A:264:MET:CE	2.42	0.49
1:A:267:GLN:O	1:A:268:GLU:C	2.55	0.49
1:A:144:LEU:HD23	1:A:147:LEU:HD12	1.95	0.49
1:A:233:LYS:HB2	5:A:672:HOH:O	2.12	0.48
1:A:142:ARG:HD2	5:A:648:HOH:O	2.13	0.48
1:A:209:HIS:O	1:A:213:CYS:SG	2.57	0.48
1:A:208:ASN:HB3	1:A:363:ILE:HD11	1.94	0.48
1:A:44:TRP:CD1	1:A:157:PRO:HG2	2.49	0.48
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.76	0.47
1:A:43:GLN:NE2	1:A:157:PRO:HG3	2.28	0.47
1:A:298:MET:CG	5:A:652:HOH:O	2.61	0.47
1:A:186:ILE:HG12	5:A:678:HOH:O	2.15	0.47
1:A:171:GLU:HG2	5:A:710:HOH:O	2.15	0.46
1:A:254:ALA:HB1	1:A:256:ASP:OD1	2.15	0.46
1:A:193:LYS:HD3	1:A:396:TYR:CZ	2.51	0.46
1:A:38:HIS:HB3	1:A:403:ALA:CB	2.45	0.46
1:A:177:ASP:CG	5:A:647:HOH:O	2.57	0.46
1:A:238:HIS:CE1	1:A:265:PRO:HB3	2.50	0.46
1:A:59:TYR:HB3	1:A:72:VAL:HG12	1.96	0.45
1:A:79:VAL:O	1:A:141:LEU:HD22	2.17	0.45
1:A:177:ASP:OD1	1:A:336:LYS:NZ	2.32	0.45
1:A:361:ARG:O	1:A:362:GLU:C	2.59	0.45
1:A:332:TRP:NE1	1:A:350:THR:HG22	2.32	0.45
1:A:165:LEU:HD22	1:A:252:VAL:HG11	1.97	0.45
1:A:171:GLU:HG3	1:A:172:VAL:N	2.32	0.45
1:A:219:ASP:O	1:A:221:GLU:N	2.50	0.45
1:A:305:TRP:C	1:A:306:ASN:ND2	2.75	0.45
1:A:296:LEU:HB3	1:A:308:PHE:HB2	1.98	0.44
1:A:394:ASP:HB2	5:A:646:HOH:O	2.17	0.44
1:A:234:LYS:N	5:A:606:HOH:O	2.39	0.44
1:A:117:GLY:O	1:A:118:LYS:C	2.59	0.44
1:A:45:LEU:HD22	1:A:303:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:THR:O	1:A:315:THR:OG1	2.35	0.44
1:A:315:THR:OG1	1:A:331:THR:HB	2.18	0.43
1:A:316:PHE:HE1	5:A:605:HOH:O	2.00	0.43
1:A:177:ASP:CB	5:A:647:HOH:O	2.66	0.43
1:A:30:GLU:O	1:A:34:LEU:HG	2.18	0.43
1:A:365:GLU:O	1:A:369:GLN:HG3	2.18	0.43
1:A:172:VAL:HG23	1:A:173:HIS:CD2	2.54	0.43
1:A:373:SER:C	1:A:375:ALA:N	2.77	0.43
1:A:75:ARG:C	1:A:77:GLY:H	2.27	0.43
1:A:209:HIS:CE1	1:A:359:GLU:HB2	2.54	0.42
1:A:191:ASN:OD1	1:A:193:LYS:HB2	2.19	0.42
1:A:217:PRO:HB3	1:A:222:VAL:HG21	1.99	0.42
1:A:110:GLN:N	1:A:110:GLN:CD	2.78	0.42
1:A:356:THR:OG1	5:A:602:HOH:O	2.14	0.42
1:A:313:SER:HB2	1:A:333:LEU:HB2	2.00	0.42
1:A:193:LYS:HD3	1:A:396:TYR:CE2	2.55	0.41
1:A:278:LYS:HE2	1:A:278:LYS:HB3	1.99	0.41
1:A:258:GLN:HB2	5:A:650:HOH:O	2.19	0.41
1:A:314:LEU:N	5:A:612:HOH:O	2.53	0.41
1:A:46:TYR:OH	1:A:315:THR:CG2	2.60	0.41
1:A:252:VAL:HG23	5:A:688:HOH:O	2.20	0.41
1:A:306:ASN:ND2	1:A:306:ASN:N	2.69	0.41
1:A:49:PRO:HG3	1:A:333:LEU:HD21	2.03	0.40
1:A:212:LEU:O	1:A:215:SER:N	2.45	0.40
1:A:76:ASP:OD2	1:A:76:ASP:C	2.64	0.40
1:A:298:MET:O	1:A:305:TRP:HA	2.21	0.40
1:A:23:GLN:N	5:A:616:HOH:O	2.54	0.40
1:A:282:SER:HB3	5:A:697:HOH:O	2.22	0.40
1:A:290:PRO:HB2	1:A:291:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	393/412 (95%)	348 (88%)	38 (10%)	7 (2%)	6 4

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ALA
1	A	76	ASP
1	A	203	TYR
1	A	269	LYS
1	A	205	CYS
1	A	268	GLU
1	A	95	LYS

5.3.2 Protein sidechains (i)

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	337/349 (97%)	309 (92%)	28 (8%)	10 11

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLU
1	A	75	ARG
1	A	100	GLN
1	A	118	LYS
1	A	137	LYS
1	A	147	LEU
1	A	171	GLU
1	A	176	LYS
1	A	179	LYS
1	A	202	CYS
1	A	215	SER
1	A	218	LEU
1	A	219	ASP
1	A	221	GLU

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Mol	Chain	Res	Type
1	A	222	VAL
1	A	233	LYS
1	A	252	VAL
1	A	260	ARG
1	A	271	LEU
1	A	275	MET
1	A	278	LYS
1	A	281	VAL
1	A	283	ARG
1	A	298	MET
1	A	306	ASN
1	A	313	SER
1	A	342	VAL
1	A	361	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	98	GLN
1	A	100	GLN
1	A	198	ASN
1	A	267	GLN
1	A	306	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	NCO	A	503	-	6,6,6	0.43	0	-		
2	FES	A	501	1	0,4,4	-	-	-		

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
2	FES	A	501	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FES	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	397/412 (96%)	1.38	86 (21%)	2 1	9, 23, 46, 69	1 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	LEU	8.1
1	A	216	PHE	5.8
1	A	18	GLY	5.3
1	A	405	ALA	5.2
1	A	220	PRO	5.0
1	A	221	GLU	4.5
1	A	406	PRO	4.5
1	A	205	CYS	4.4
1	A	217	PRO	4.2
1	A	224	GLY	4.0
1	A	268	GLU	3.9
1	A	219	ASP	3.8
1	A	204	HIS	3.7
1	A	209	HIS	3.7
1	A	225	VAL	3.7
1	A	222	VAL	3.6
1	A	210	PRO	3.6
1	A	77	GLY	3.6
1	A	214	ARG	3.6
1	A	127	PRO	3.6
1	A	215	SER	3.5
1	A	118	LYS	3.5
1	A	291	PRO	3.5
1	A	206	SER	3.5
1	A	283	ARG	3.4
1	A	75	ARG	3.4
1	A	223	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	54	ALA	3.2
1	A	97	ARG	3.2
1	A	212	LEU	3.2
1	A	55	LYS	3.1
1	A	207	SER	3.1
1	A	128	ASP	3.0
1	A	213	CYS	3.0
1	A	76	ASP	3.0
1	A	277	GLY	2.9
1	A	293	ALA	2.9
1	A	285	LEU	2.9
1	A	203	TYR	2.8
1	A	123	ASN	2.8
1	A	276	ASP	2.8
1	A	208	ASN	2.8
1	A	404	LEU	2.7
1	A	252	VAL	2.7
1	A	241	ARG	2.6
1	A	287	ARG	2.6
1	A	402	ARG	2.6
1	A	288	VAL	2.6
1	A	246	GLY	2.6
1	A	202	CYS	2.6
1	A	282	SER	2.5
1	A	234	LYS	2.5
1	A	237	ALA	2.5
1	A	256	ASP	2.5
1	A	230	GLY	2.5
1	A	267	GLN	2.5
1	A	231	VAL	2.5
1	A	339	VAL	2.4
1	A	269	LYS	2.4
1	A	311	ASP	2.4
1	A	49	PRO	2.4
1	A	265	PRO	2.3
1	A	96	ALA	2.3
1	A	17	SER	2.3
1	A	79	VAL	2.3
1	A	78	GLU	2.3
1	A	113	TYR	2.3
1	A	6	THR	2.3
1	A	129	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	156	PRO	2.3
1	A	8	ILE	2.3
1	A	254	ALA	2.2
1	A	232	SER	2.2
1	A	160	GLN	2.2
1	A	122	ALA	2.1
1	A	261	LEU	2.1
1	A	154	ASP	2.1
1	A	126	GLY	2.1
1	A	120	ILE	2.1
1	A	159	PHE	2.1
1	A	132	SER	2.1
1	A	271	LEU	2.1
1	A	9	HIS	2.0
1	A	16	LEU	2.0
1	A	297	LEU	2.0
1	A	363	ILE	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(Å^2)	Q<0.9
3	FE	A	502	1/1	0.88	0.10	52,52,52,52	0
4	NCO	A	503	7/7	0.98	0.08	20,21,22,22	7
2	FES	A	501	4/4	0.99	0.04	16,17,18,19	0

6.5 Other polymers (i)

There are no such residues in this entry.