Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:27 AM GMT

PDB ID	:	3EQQ
Title	:	Apo Toluene 2,3-Dioxygenase
Authors	:	Friemann, R.; Lee, K; Brown, E.N.; Gibson, D.T.; Eklund, H.; Ramaswamy, S.
Deposited on	:	2008-10-01
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

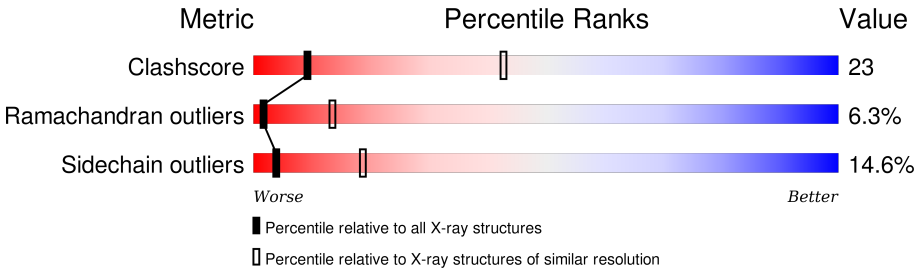
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	FAILED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	450	55% 26% 10% • 8%
2	B	187	54% 27% 13% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	A	451	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4826 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.

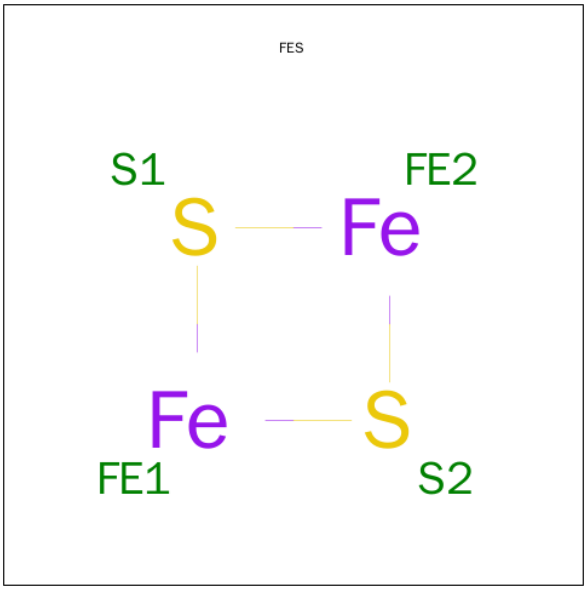
- Molecule 1 is a protein called Benzene 1,2-dioxygenase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3322	2100	576	626	20			

- Molecule 2 is a protein called Benzene 1,2-dioxygenase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1499	947	267	280	5			

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Fe 1 1	0	0

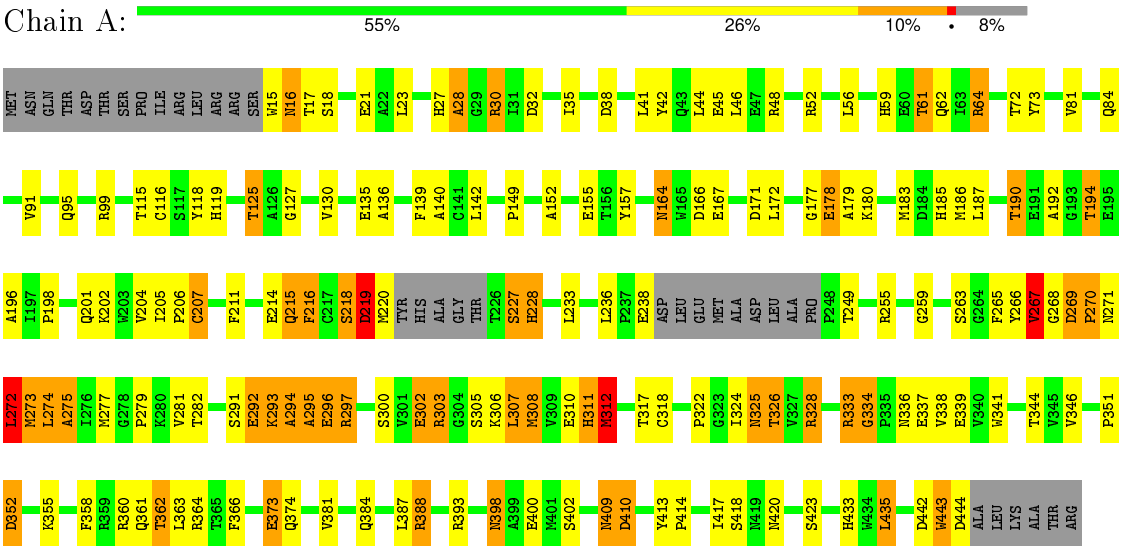
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS failed to run properly.

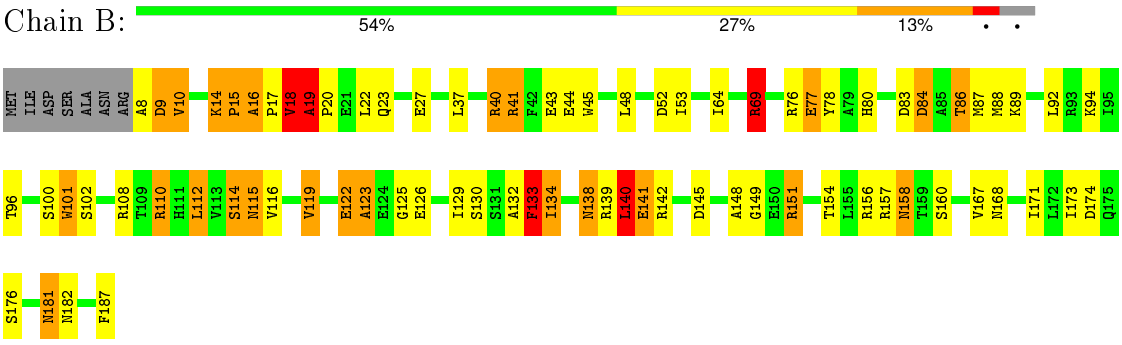
- Molecule 1: Benzene 1,2-dioxygenase subunit alpha

Chain A:



- Molecule 2: Benzene 1,2-dioxygenase subunit beta

Chain B:



4 Data and refinement statistics (i)

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α, β, γ	235.87Å 235.87Å 235.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 3.20	Depositor
% Data completeness (in resolution range)	95.7 (48.17-3.20)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.245 , 0.279	Depositor
Wilson B-factor (Å^2)	83.0	Xtriage
Anisotropy	0.000	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
Outliers	0 of 35920 reflections	Xtriage
Total number of atoms	4826	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: FE2, FES

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	0.77	0/3413	0.85	5/4634 (0.1%)
2	B	0.85	0/1532	0.95	8/2067 (0.4%)
All	All	0.79	0/4945	0.88	13/6701 (0.2%)

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	4
2	B	0	3
All	All	0	7

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	333	ARG	NE-CZ-NH1	7.00	123.80	120.30
2	B	19	ALA	N-CA-C	-6.55	93.31	111.00
2	B	16	ALA	N-CA-C	-6.48	93.50	111.00
2	B	112	LEU	CA-CB-CG	-6.23	100.97	115.30
2	B	133	PHE	N-CA-C	6.11	127.50	111.00
1	A	333	ARG	NE-CZ-NH2	-6.03	117.29	120.30
2	B	125	GLY	N-CA-C	-5.80	98.60	113.10
1	A	274	LEU	CA-CB-CG	5.72	128.45	115.30
1	A	233	LEU	CA-CB-CG	5.61	128.20	115.30
2	B	114	SER	N-CA-C	5.52	125.92	111.00
1	A	272	LEU	CA-CB-CG	5.19	127.24	115.30
2	B	83	ASP	CB-CG-OD2	5.05	122.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	84	ASP	CB-CA-C	-5.03	100.33	110.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	GLU	Peptide
1	A	219	ASP	Peptide
1	A	227	SER	Peptide
1	A	334	GLY	Peptide
2	B	123	ALA	Peptide
2	B	132	ALA	Peptide
2	B	18	VAL	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	3322	0	3149	143	0
2	B	1499	0	1451	81	0
3	A	4	0	0	3	0
4	B	1	0	0	0	0
All	All	4826	0	4600	216	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 23.

All (216) 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:207:CYS:HA	1:A:384:GLN:HG3	1.18	1.16
1:A:269:ASP:HB2	1:A:270:PRO:HD2	1.18	1.14
2:B:19:ALA:HB3	2:B:20:PRO:HA	1.31	1.06
2:B:14:LYS:H	2:B:14:LYS:HD2	1.21	1.02
1:A:291:SER:O	1:A:295:ALA:HB3	1.62	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PHE:HD1	1:A:216:PHE:H	1.02	0.95
1:A:116:CYS:HG	3:A:451:FES:FE2	0.83	0.92
1:A:296:GLU:HA	1:A:296:GLU:OE2	1.67	0.92
2:B:19:ALA:HB3	2:B:20:PRO:CA	2.00	0.92
2:B:108:ARG:HE	2:B:138:ASN:ND2	1.67	0.91
1:A:344:THR:OG1	1:A:362:THR:HG21	1.72	0.90
2:B:139:ARG:NH2	2:B:181:ASN:HD21	1.73	0.85
1:A:216:PHE:HD1	1:A:216:PHE:N	1.76	0.84
1:A:269:ASP:HB2	1:A:270:PRO:CD	2.06	0.83
2:B:158:ASN:HD22	2:B:160:SER:H	1.24	0.82
1:A:205:ILE:HG23	1:A:205:ILE:O	1.78	0.82
1:A:164:ASN:ND2	1:A:166:ASP:H	1.77	0.82
1:A:205:ILE:CG2	1:A:338:VAL:HG12	2.09	0.81
2:B:15:PRO:HB2	2:B:16:ALA:HA	1.62	0.81
2:B:14:LYS:H	2:B:14:LYS:CD	1.94	0.80
2:B:139:ARG:HH22	2:B:181:ASN:ND2	1.81	0.79
1:A:227:SER:O	1:A:228:HIS:HB2	1.84	0.78
1:A:269:ASP:CB	1:A:270:PRO:HD2	2.07	0.77
2:B:15:PRO:HB2	2:B:16:ALA:CA	2.14	0.77
1:A:207:CYS:CA	1:A:384:GLN:HG3	2.06	0.77
1:A:201:GLN:HE21	2:B:80:HIS:HD2	1.32	0.77
1:A:294:ALA:O	1:A:297:ARG:HG3	1.86	0.75
1:A:164:ASN:HD22	1:A:166:ASP:H	1.32	0.73
1:A:186:MET:HB2	1:A:322:PRO:HB3	1.70	0.72
2:B:108:ARG:HE	2:B:138:ASN:HD22	1.38	0.72
1:A:328:ARG:NH1	1:A:373:GLU:OE2	2.22	0.72
2:B:139:ARG:NH2	2:B:181:ASN:ND2	2.36	0.71
1:A:84:GLN:OE1	1:A:125:THR:HG22	1.90	0.71
1:A:64:ARG:HG2	1:A:64:ARG:HH11	1.55	0.71
1:A:277:MET:HA	1:A:361:GLN:HG2	1.72	0.71
2:B:19:ALA:HB1	2:B:22:LEU:HB3	1.72	0.70
1:A:119:HIS:HB2	3:A:451:FES:S1	2.31	0.70
1:A:205:ILE:HG22	1:A:338:VAL:O	1.92	0.70
1:A:205:ILE:CG2	1:A:205:ILE:O	2.39	0.70
1:A:310:GLU:HB3	1:A:322:PRO:HG2	1.73	0.70
2:B:14:LYS:HD2	2:B:14:LYS:N	2.03	0.69
1:A:266:TYR:O	1:A:267:VAL:HG13	1.92	0.69
1:A:302:GLU:HA	1:A:306:LYS:HB2	1.73	0.69
1:A:116:CYS:SG	3:A:451:FES:FE2	1.86	0.67
1:A:205:ILE:HG23	1:A:338:VAL:HG12	1.76	0.67
1:A:269:ASP:O	1:A:308:MET:HE2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:PHE:O	1:A:215:GLN:HB2	1.95	0.66
2:B:10:VAL:HG13	2:B:119:VAL:HG21	1.78	0.66
1:A:21:GLU:HA	1:A:435:LEU:HD21	1.77	0.66
1:A:302:GLU:HG3	1:A:303:ARG:N	2.11	0.66
1:A:15:TRP:O	1:A:16:ASN:CB	2.43	0.66
2:B:133:PHE:HD2	2:B:148:ALA:C	1.99	0.66
2:B:154:THR:HB	2:B:168:ASN:HB2	1.78	0.66
2:B:9:ASP:O	2:B:10:VAL:HB	1.96	0.65
1:A:202:LYS:HD3	1:A:341:TRP:CE2	2.31	0.65
1:A:442:ASP:O	1:A:443:TRP:HB2	1.97	0.65
2:B:133:PHE:HB2	2:B:149:GLY:O	1.97	0.65
2:B:149:GLY:HA2	2:B:174:ASP:OD2	1.97	0.64
2:B:19:ALA:CB	2:B:23:GLN:H	2.11	0.64
2:B:84:ASP:HB3	2:B:86:THR:H	1.62	0.63
1:A:205:ILE:CG2	1:A:338:VAL:CG1	2.76	0.63
1:A:311:HIS:O	1:A:312:MET:HB2	1.99	0.63
1:A:417:ILE:N	1:A:417:ILE:HD12	2.14	0.62
2:B:69:ARG:NH1	2:B:69:ARG:HB3	2.13	0.62
2:B:92:LEU:O	2:B:96:THR:HG23	1.99	0.62
2:B:69:ARG:H	2:B:69:ARG:HD2	1.65	0.61
1:A:358:PHE:O	1:A:362:THR:HB	2.02	0.60
1:A:324:ILE:O	1:A:325:ASN:HB2	1.99	0.60
1:A:387:LEU:O	1:A:393:ARG:HD2	2.01	0.60
1:A:185:HIS:NE2	1:A:303:ARG:HD3	2.16	0.60
1:A:362:THR:HG22	2:B:78:TYR:HE1	1.67	0.59
1:A:274:LEU:O	1:A:275:ALA:HB3	2.03	0.59
2:B:19:ALA:CB	2:B:20:PRO:CA	2.79	0.59
1:A:61:THR:HG21	1:A:196:ALA:O	2.03	0.58
2:B:19:ALA:CB	2:B:22:LEU:HB3	2.33	0.58
1:A:216:PHE:N	1:A:216:PHE:CD1	2.48	0.58
2:B:9:ASP:O	2:B:10:VAL:CB	2.52	0.57
1:A:81:VAL:HG22	1:A:91:VAL:HG22	1.86	0.57
1:A:272:LEU:HD23	1:A:308:MET:HA	1.85	0.57
1:A:190:THR:HG23	1:A:192:ALA:H	1.70	0.57
1:A:291:SER:O	1:A:295:ALA:CB	2.47	0.56
1:A:44:LEU:HD13	1:A:48:ARG:HH21	1.68	0.56
1:A:202:LYS:HD3	1:A:341:TRP:CD2	2.41	0.56
1:A:206:PRO:HA	1:A:337:GLU:HA	1.87	0.56
2:B:41:ARG:HD2	2:B:44:GLU:OE1	2.05	0.55
1:A:177:GLY:O	1:A:180:LYS:HE2	2.07	0.55
1:A:164:ASN:HD22	1:A:166:ASP:N	2.02	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:ASN:HD22	2:B:181:ASN:H	1.55	0.54
2:B:17:PRO:O	2:B:18:VAL:HG22	2.06	0.54
1:A:30:ARG:NH2	1:A:400:GLU:OE2	2.41	0.54
1:A:273:MET:HA	1:A:282:THR:OG1	2.08	0.54
1:A:334:GLY:C	1:A:336:ASN:H	2.11	0.54
2:B:140:LEU:O	2:B:141:GLU:HB2	2.07	0.54
1:A:64:ARG:HG2	1:A:64:ARG:NH1	2.22	0.54
1:A:219:ASP:OD1	1:A:219:ASP:N	2.40	0.54
1:A:263:SER:HB2	1:A:312:MET:HG2	1.90	0.53
2:B:122:GLU:O	2:B:123:ALA:HB3	2.08	0.53
1:A:211:PHE:O	1:A:215:GLN:CB	2.56	0.53
1:A:16:ASN:HD21	1:A:18:SER:HB3	1.74	0.53
1:A:204:VAL:O	2:B:181:ASN:HA	2.08	0.52
1:A:360:ARG:HE	2:B:87:MET:HE2	1.74	0.52
1:A:346:VAL:HG21	1:A:355:LYS:HG2	1.90	0.52
2:B:100:SER:HB2	2:B:101:TRP:HD1	1.74	0.52
1:A:270:PRO:HB3	1:A:274:LEU:HD12	1.92	0.52
1:A:293:LYS:O	1:A:295:ALA:N	2.42	0.52
2:B:133:PHE:CE1	2:B:151:ARG:HD2	2.44	0.51
2:B:171:ILE:HD13	2:B:187:PHE:HB2	1.92	0.51
2:B:115:ASN:N	2:B:115:ASN:ND2	2.58	0.51
2:B:27:GLU:HG2	2:B:116:VAL:HG21	1.93	0.51
2:B:158:ASN:ND2	2:B:160:SER:H	2.02	0.51
1:A:387:LEU:O	1:A:393:ARG:CD	2.59	0.51
1:A:157:TYR:OH	1:A:180:LYS:HB3	2.11	0.51
2:B:84:ASP:HB3	2:B:86:THR:N	2.26	0.50
2:B:88:MET:O	2:B:89:LYS:C	2.50	0.50
1:A:273:MET:O	1:A:274:LEU:C	2.49	0.50
2:B:8:ALA:O	2:B:9:ASP:HB2	2.11	0.50
1:A:333:ARG:NH1	1:A:339:GLU:OE2	2.45	0.50
1:A:265:PHE:HB3	1:A:310:GLU:HG3	1.94	0.50
1:A:201:GLN:HE21	2:B:80:HIS:CD2	2.21	0.50
1:A:56:LEU:HD22	1:A:318:CYS:SG	2.51	0.50
2:B:15:PRO:HB2	2:B:16:ALA:CB	2.41	0.49
2:B:116:VAL:O	2:B:116:VAL:HG23	2.12	0.49
1:A:139:PHE:HB3	1:A:142:LEU:HB2	1.94	0.49
2:B:108:ARG:HE	2:B:138:ASN:HD21	1.52	0.49
1:A:42:TYR:HA	1:A:45:GLU:HG3	1.95	0.49
1:A:127:GLY:O	1:A:149:PRO:HD2	2.13	0.48
1:A:211:PHE:HE1	1:A:384:GLN:HE21	1.61	0.48
1:A:91:VAL:HG12	1:A:152:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:PRO:CB	2:B:16:ALA:CA	2.90	0.48
1:A:402:SER:HB2	1:A:423:SER:HB2	1.96	0.48
2:B:151:ARG:NH1	2:B:187:PHE:OXT	2.44	0.48
1:A:417:ILE:H	1:A:417:ILE:HD12	1.79	0.48
1:A:373:GLU:HG3	1:A:373:GLU:O	2.14	0.48
1:A:388:ARG:HG3	1:A:388:ARG:HH11	1.78	0.48
1:A:388:ARG:HG3	1:A:388:ARG:NH1	2.29	0.48
1:A:300:SER:HB3	1:A:303:ARG:HB2	1.95	0.47
2:B:158:ASN:ND2	2:B:160:SER:OG	2.48	0.47
2:B:45:TRP:O	2:B:48:LEU:HB2	2.15	0.47
1:A:185:HIS:NE2	1:A:303:ARG:CD	2.77	0.47
1:A:218:SER:O	1:A:220:MET:N	2.48	0.47
2:B:84:ASP:HB2	2:B:87:MET:HE3	1.96	0.47
1:A:268:GLY:O	1:A:269:ASP:CB	2.63	0.47
2:B:10:VAL:HG13	2:B:119:VAL:CG2	2.43	0.46
1:A:398:ASN:ND2	1:A:400:GLU:H	2.12	0.46
1:A:35:ILE:HA	1:A:41:LEU:HD23	1.97	0.46
1:A:272:LEU:HG	1:A:282:THR:HG23	1.97	0.46
1:A:179:ALA:O	1:A:183:MET:HG3	2.15	0.46
2:B:110:ARG:HA	2:B:110:ARG:HD3	1.52	0.46
1:A:328:ARG:NH2	1:A:366:PHE:O	2.48	0.46
2:B:84:ASP:H	2:B:87:MET:HE3	1.80	0.46
1:A:274:LEU:O	1:A:275:ALA:CB	2.64	0.46
1:A:294:ALA:O	1:A:296:GLU:N	2.49	0.46
1:A:326:THR:HG21	1:A:328:ARG:HH21	1.79	0.46
2:B:171:ILE:CD1	2:B:187:PHE:HB2	2.46	0.46
1:A:155:GLU:OE2	1:A:172:LEU:HB3	2.16	0.46
2:B:157:ARG:HG2	2:B:157:ARG:NH1	2.31	0.46
1:A:15:TRP:O	1:A:16:ASN:HB3	2.16	0.46
1:A:72:THR:OG1	1:A:73:TYR:N	2.49	0.46
1:A:259:GLY:HA2	1:A:433:HIS:CE1	2.50	0.46
1:A:442:ASP:O	1:A:443:TRP:CB	2.64	0.45
1:A:32:ASP:C	1:A:32:ASP:OD1	2.53	0.45
1:A:300:SER:CB	1:A:303:ARG:HB2	2.45	0.45
1:A:164:ASN:C	1:A:164:ASN:HD22	2.19	0.45
1:A:351:PRO:O	1:A:352:ASP:C	2.54	0.45
2:B:18:VAL:HG23	2:B:19:ALA:HB2	1.99	0.45
1:A:300:SER:OG	1:A:303:ARG:HB2	2.15	0.45
1:A:362:THR:HG22	1:A:363:LEU:N	2.31	0.45
2:B:126:GLU:OE1	2:B:156:ARG:HD3	2.17	0.44
2:B:173:ILE:HA	2:B:173:ILE:HD12	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:ASP:O	2:B:88:MET:HG2	2.18	0.44
1:A:334:GLY:C	1:A:336:ASN:N	2.69	0.44
1:A:41:LEU:HD12	1:A:41:LEU:HA	1.75	0.44
2:B:133:PHE:CD2	2:B:149:GLY:N	2.85	0.44
2:B:157:ARG:HH11	2:B:157:ARG:HG2	1.83	0.44
1:A:307:LEU:HD23	1:A:307:LEU:HA	1.66	0.44
1:A:362:THR:CG2	2:B:78:TYR:HE1	2.28	0.43
2:B:133:PHE:HD2	2:B:149:GLY:N	2.15	0.43
1:A:409:ASN:O	1:A:410:ASP:O	2.36	0.43
1:A:211:PHE:O	1:A:215:GLN:HG3	2.18	0.43
1:A:15:TRP:O	1:A:16:ASN:HB2	2.17	0.43
1:A:268:GLY:O	1:A:269:ASP:CG	2.57	0.43
2:B:115:ASN:N	2:B:115:ASN:HD22	2.15	0.43
1:A:334:GLY:CA	1:A:336:ASN:H	2.32	0.43
1:A:409:ASN:O	1:A:410:ASP:C	2.57	0.43
1:A:164:ASN:ND2	1:A:166:ASP:N	2.57	0.43
2:B:114:SER:O	2:B:116:VAL:N	2.52	0.43
2:B:182:ASN:OD1	2:B:182:ASN:C	2.57	0.43
1:A:59:HIS:H	1:A:62:GLN:NE2	2.17	0.43
1:A:187:LEU:HD23	1:A:194:THR:HG21	2.01	0.43
2:B:84:ASP:H	2:B:87:MET:CE	2.31	0.43
1:A:334:GLY:HA3	1:A:336:ASN:H	1.83	0.43
1:A:46:LEU:HA	1:A:46:LEU:HD23	1.80	0.43
1:A:388:ARG:HD2	1:A:388:ARG:HA	1.70	0.42
2:B:129:ILE:CG2	2:B:130:SER:N	2.81	0.42
2:B:52:ASP:OD1	2:B:52:ASP:N	2.53	0.42
1:A:398:ASN:C	1:A:398:ASN:HD22	2.23	0.42
1:A:292:GLU:C	1:A:293:LYS:O	2.58	0.42
1:A:23:LEU:HD13	1:A:35:ILE:HG22	2.01	0.42
2:B:40:ARG:HB2	2:B:40:ARG:HE	1.73	0.42
2:B:53:ILE:HG23	2:B:53:ILE:O	2.20	0.42
1:A:413:TYR:HA	1:A:414:PRO:HD3	1.94	0.42
1:A:27:HIS:O	1:A:28:ALA:CB	2.68	0.42
1:A:52:ARG:HG2	1:A:166:ASP:OD1	2.20	0.41
1:A:402:SER:CB	1:A:423:SER:HB2	2.49	0.41
1:A:215:GLN:HB3	1:A:216:PHE:HA	2.02	0.41
2:B:19:ALA:HB1	2:B:23:GLN:H	1.84	0.41
1:A:38:ASP:HB3	1:A:41:LEU:HB2	2.02	0.41
2:B:133:PHE:HE1	2:B:151:ARG:HD2	1.84	0.41
1:A:398:ASN:ND2	1:A:398:ASN:C	2.74	0.41
2:B:101:TRP:N	2:B:101:TRP:CD1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PRO:HG2	1:A:381:VAL:HG13	2.03	0.40
1:A:198:PRO:HG2	2:B:77:GLU:HB3	2.01	0.40
1:A:99:ARG:HA	1:A:99:ARG:HD3	1.94	0.40
1:A:364:ARG:HD3	2:B:87:MET:HG2	2.04	0.40
1:A:333:ARG:HD2	1:A:339:GLU:OE2	2.22	0.40
1:A:326:THR:HB	1:A:328:ARG:HE	1.87	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	410/450 (91%)	336 (82%)	47 (12%)	27 (7%)	1 12
2	B	178/187 (95%)	150 (84%)	18 (10%)	10 (6%)	2 18
All	All	588/637 (92%)	486 (83%)	65 (11%)	37 (6%)	2 13

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	171	ASP
1	A	269	ASP
1	A	270	PRO
1	A	271	ASN
1	A	273	MET
1	A	275	ALA
1	A	293	LYS
1	A	294	ALA
2	B	10	VAL
2	B	15	PRO
2	B	19	ALA

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Mol	Chain	Res	Type
2	B	69	ARG
2	B	134	ILE
1	A	17	THR
1	A	28	ALA
1	A	136	ALA
1	A	215	GLN
1	A	219	ASP
1	A	267	VAL
1	A	295	ALA
1	A	352	ASP
2	B	18	VAL
1	A	125	THR
1	A	292	GLU
1	A	311	HIS
1	A	443	TRP
2	B	9	ASP
1	A	140	ALA
2	B	141	GLU
2	B	176	SER
1	A	279	PRO
1	A	312	MET
1	A	325	ASN
1	A	410	ASP
2	B	140	LEU
1	A	178	GLU

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	348/376 (93%)	302 (87%)	46 (13%)	5 23
2	B	159/165 (96%)	131 (82%)	28 (18%)	2 11
All	All	507/541 (94%)	433 (85%)	74 (15%)	4 19

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	61	THR
1	A	64	ARG
1	A	95	GLN
1	A	115	THR
1	A	118	TYR
1	A	130	VAL
1	A	135	GLU
1	A	164	ASN
1	A	167	GLU
1	A	178	GLU
1	A	190	THR
1	A	194	THR
1	A	207	CYS
1	A	216	PHE
1	A	218	SER
1	A	219	ASP
1	A	228	HIS
1	A	236	LEU
1	A	238	GLU
1	A	249	THR
1	A	255	ARG
1	A	267	VAL
1	A	272	LEU
1	A	281	VAL
1	A	296	GLU
1	A	297	ARG
1	A	302	GLU
1	A	303	ARG
1	A	305	SER
1	A	307	LEU
1	A	308	MET
1	A	312	MET
1	A	317	THR
1	A	326	THR
1	A	328	ARG
1	A	362	THR
1	A	373	GLU
1	A	374	GLN
1	A	388	ARG
1	A	398	ASN
1	A	409	ASN
1	A	418	SER

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Mol	Chain	Res	Type
1	A	420	ASN
1	A	435	LEU
1	A	444	ASP
2	B	14	LYS
2	B	37	LEU
2	B	40	ARG
2	B	41	ARG
2	B	43	GLU
2	B	64	ILE
2	B	69	ARG
2	B	76	ARG
2	B	77	GLU
2	B	86	THR
2	B	94	LYS
2	B	101	TRP
2	B	102	SER
2	B	110	ARG
2	B	112	LEU
2	B	115	ASN
2	B	119	VAL
2	B	122	GLU
2	B	133	PHE
2	B	134	ILE
2	B	138	ASN
2	B	140	LEU
2	B	142	ARG
2	B	145	ASP
2	B	151	ARG
2	B	158	ASN
2	B	167	VAL
2	B	181	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	62	GLN
1	A	164	ASN
1	A	331	HIS
1	A	384	GLN
1	A	398	ASN
1	A	409	ASN

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Mol	Chain	Res	Type
1	A	420	ASN
2	B	38	ASN
2	B	80	HIS
2	B	115	ASN
2	B	138	ASN
2	B	143	GLN
2	B	158	ASN
2	B	168	ASN
2	B	181	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\#\|Z\| > 2$
3	FES	A	451	1	0,4,4	0.00	-	0,4,4	0.00	-

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
3	FES	A	451	1	-	0/0/4/4	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	451	FES	3	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

EDS failed to run properly - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers

EDS failed to run properly - this section will therefore be empty.