



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:03 AM GMT

PDB ID : 4HGV
Title : Crystal structure of a fumarate hydratase
Authors : Eswaramoorthy, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; Lafleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)
Deposited on : 2012-10-08
Resolution : 2.09 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

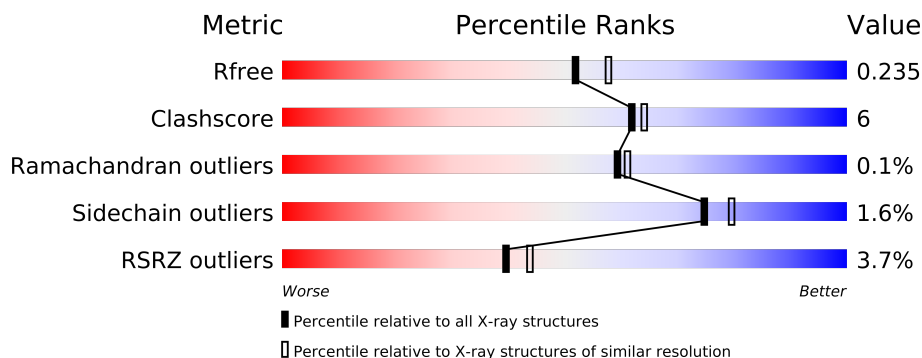
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.09 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	495	
1	B	495	
1	C	495	
1	D	495	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	D	501	-	X

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 13548 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Fumarate hydratase class II.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	Se	0	0	0
			3388	2124	596	653	5	10			
1	B	453	Total	C	N	O	S	Se	0	0	0
			3388	2128	595	650	5	10			
1	C	411	Total	C	N	O	S	Se	0	0	0
			3060	1923	536	586	5	10			
1	D	454	Total	C	N	O	S	Se	0	0	0
			3381	2121	593	651	5	11			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

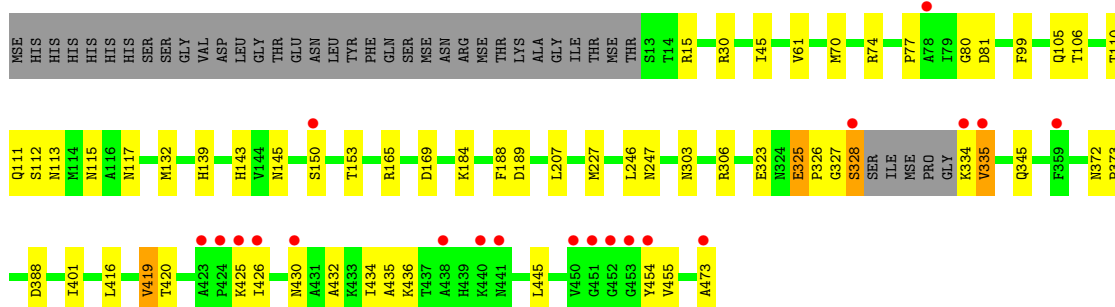
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	82	Total	O	0	0
			82	82		
3	C	77	Total	O	0	0
			77	77		
3	D	80	Total	O	0	0
			80	80		

3 Residue-property plots

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.

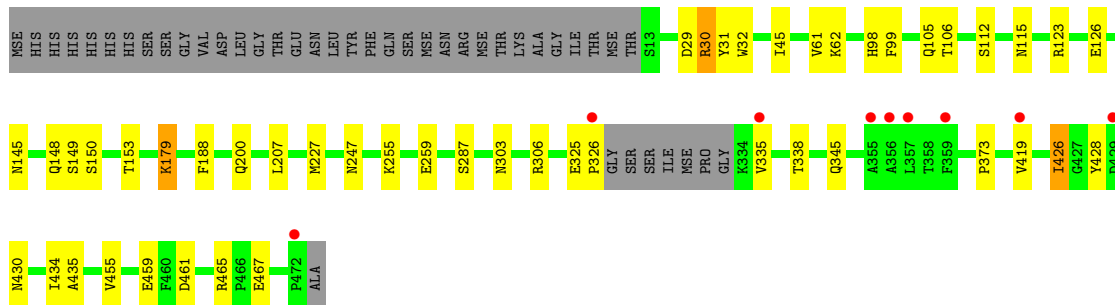
• Molecule 1: Fumarate hydratase class II

Chain A:



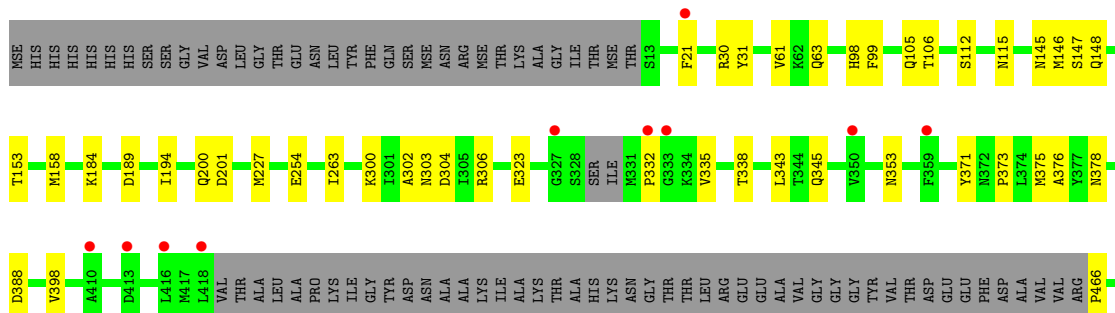
• Molecule 1: Fumarate hydratase class II

Chain B:



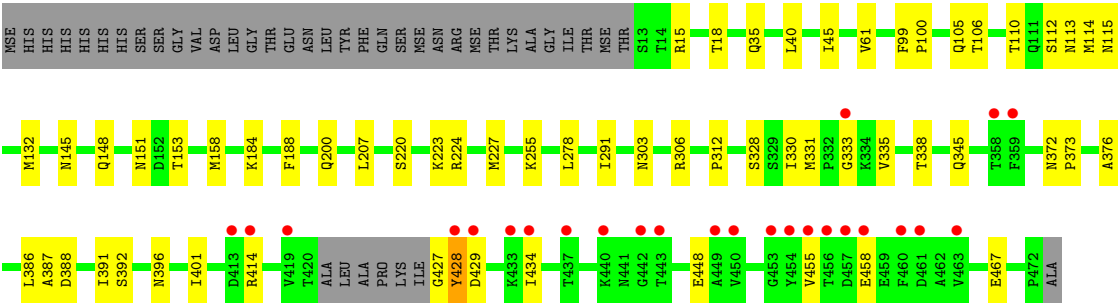
• Molecule 1: Fumarate hydratase class II

Chain C:





● Molecule 1: Fumarate hydratase class II



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.16Å 159.97Å 162.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.76 – 2.09 44.76 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.0 (44.76-2.09) 99.1 (44.76-2.09)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.197 , 0.234 0.200 , 0.235	Depositor DCC
R_{free} test set	5494 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 25.9	EDS
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 110245 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13548	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 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.50	0/3439	0.58	0/4653
1	B	0.50	0/3440	0.57	0/4652
1	C	0.52	0/3107	0.57	0/4199
1	D	0.52	0/3432	0.57	0/4640
All	All	0.51	0/13418	0.57	0/18144

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3388	0	3352	54	0
1	B	3388	0	3368	43	0
1	C	3060	0	3031	38	0
1	D	3381	0	3341	44	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
3	A	77	0	0	0	0
3	B	82	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	77	0	0	1	0
3	D	80	0	0	1	0
All	All	13548	0	13092	150	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (150) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:70:MSE:HE3	1:A:80:GLY:HA3	1.26	1.12
1:A:70:MSE:HE2	1:A:77:PRO:HA	1.17	1.09
1:A:70:MSE:CE	1:A:77:PRO:HA	1.95	0.95
1:A:70:MSE:HE3	1:A:80:GLY:CA	1.98	0.93
1:C:466:PRO:HA	1:C:469:MSE:HE3	1.50	0.92
1:A:70:MSE:HE2	1:A:77:PRO:CA	2.02	0.89
1:B:303:ASN:HD22	1:B:306:ARG:HH21	1.21	0.85
1:A:325:GLU:HG2	3:D:620:HOH:O	1.76	0.84
1:D:312:PRO:HG3	1:D:333:GLY:HA3	1.61	0.82
1:B:455:VAL:HG22	1:B:459:GLU:HB2	1.61	0.81
1:D:330:ILE:HD12	1:D:331:MSE:HG2	1.61	0.81
1:A:303:ASN:HD22	1:A:306:ARG:HH21	1.32	0.76
1:D:303:ASN:HD22	1:D:306:ARG:HH21	1.35	0.74
1:C:254:GLU:HG2	3:C:641:HOH:O	1.88	0.73
1:B:373:PRO:HD2	1:C:345:GLN:HE22	1.56	0.70
1:C:303:ASN:HD22	1:C:306:ARG:HH21	1.36	0.70
1:A:139:HIS:H	1:A:143:HIS:CD2	2.11	0.68
1:A:70:MSE:CE	1:A:80:GLY:HA3	2.15	0.68
1:D:145:ASN:O	1:D:148:GLN:HG2	1.93	0.68
1:A:105:GLN:HE22	1:A:112:SER:H	1.42	0.68
1:B:419:VAL:HG11	1:B:435:ALA:HB2	1.77	0.67
1:A:139:HIS:H	1:A:143:HIS:HD2	1.41	0.67
1:A:345:GLN:HE22	1:D:373:PRO:HD2	1.59	0.66
1:B:345:GLN:HE22	1:C:373:PRO:HD2	1.61	0.64
1:C:31:TYR:H	1:C:98:HIS:CD2	2.16	0.64
1:B:99:PHE:HA	1:B:115:ASN:HD21	1.61	0.63
1:D:61:VAL:HG11	1:D:153:THR:HG23	1.80	0.63
1:D:35:GLN:NE2	1:D:114:MSE:HG3	2.13	0.63
1:B:105:GLN:HE22	1:B:112:SER:H	1.47	0.62
1:B:29:ASP:HB3	1:B:30:ARG:HD3	1.80	0.62
1:A:70:MSE:HE1	1:A:81:ASP:N	2.14	0.62
1:B:338:THR:CG2	1:C:106:THR:HG22	2.30	0.62
1:C:194:ILE:HD11	1:C:201:ASP:HB3	1.81	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:303:ASN:ND2	1:B:306:ARG:HH21	1.95	0.60
1:A:426:ILE:HG22	1:A:430:ASN:HB2	1.83	0.60
1:A:70:MSE:HE1	1:A:81:ASP:H	1.68	0.59
1:B:106:THR:HG22	1:C:338:THR:HB	1.84	0.59
1:A:70:MSE:CE	1:A:80:GLY:CA	2.77	0.59
1:B:150:SER:HB2	3:B:511:HOH:O	2.02	0.59
1:B:338:THR:HB	1:C:106:THR:HG22	1.86	0.58
1:A:373:PRO:HD2	1:D:345:GLN:HE22	1.67	0.58
1:D:99:PHE:HA	1:D:115:ASN:HD21	1.69	0.57
1:B:326:PRO:HA	1:C:21:PHE:CD1	2.40	0.57
1:B:428:TYR:CE1	1:D:330:ILE:HG12	2.40	0.56
1:B:31:TYR:H	1:B:98:HIS:CD2	2.23	0.56
1:D:303:ASN:ND2	1:D:306:ARG:HE	2.04	0.56
1:C:105:GLN:HE22	1:C:112:SER:H	1.52	0.55
1:A:61:VAL:HG11	1:A:153:THR:HG23	1.88	0.55
1:B:145:ASN:O	1:B:148:GLN:HG2	2.07	0.55
1:B:461:ASP:O	1:B:465:ARG:HD3	2.07	0.55
1:D:105:GLN:HE22	1:D:112:SER:H	1.54	0.55
1:C:145:ASN:O	1:C:148:GLN:HG2	2.07	0.53
1:A:345:GLN:NE2	1:D:373:PRO:HD2	2.23	0.53
1:C:371:TYR:O	1:C:375:MSE:HG3	2.09	0.53
1:D:106:THR:HG21	1:D:110:THR:HB	1.92	0.52
1:A:416:LEU:O	1:A:419:VAL:HG22	2.09	0.52
1:C:466:PRO:CA	1:C:469:MSE:HE3	2.33	0.51
1:C:31:TYR:H	1:C:98:HIS:HD2	1.55	0.51
1:D:303:ASN:ND2	1:D:306:ARG:HH21	2.05	0.51
1:D:220:SER:O	1:D:224:ARG:HG3	2.10	0.51
1:B:373:PRO:HD2	1:C:345:GLN:NE2	2.24	0.51
1:A:419:VAL:HG13	1:A:445:LEU:HD22	1.92	0.51
1:A:434:ILE:HD11	1:A:454:TYR:CD1	2.45	0.51
1:B:61:VAL:HG11	1:B:153:THR:HG23	1.91	0.51
1:B:123:ARG:NH1	1:B:126:GLU:OE1	2.43	0.51
1:A:113:ASN:HD21	1:A:145:ASN:HD21	1.59	0.50
1:C:227:MSE:HG2	1:D:227:MSE:SE	2.62	0.50
1:A:45:ILE:HA	1:D:388:ASP:HB3	1.92	0.50
1:B:179:LYS:HD3	3:B:551:HOH:O	2.12	0.50
1:A:106:THR:HG22	1:D:338:THR:HB	1.93	0.49
1:A:110:THR:HA	1:A:150:SER:HB2	1.95	0.48
1:A:426:ILE:HD13	1:A:454:TYR:HB3	1.95	0.48
1:B:31:TYR:H	1:B:98:HIS:HD2	1.61	0.48
1:A:432:ALA:O	1:A:436:LYS:HG3	2.14	0.48
1:B:338:THR:CB	1:C:106:THR:HG22	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:99:PHE:HA	1:C:115:ASN:HD21	1.80	0.47
1:B:200:GLN:NE2	1:D:335:VAL:H	2.11	0.47
1:B:45:ILE:HA	1:C:388:ASP:HB3	1.97	0.47
1:A:388:ASP:HB3	1:D:45:ILE:HA	1.96	0.47
1:B:62:LYS:HZ3	1:B:148:GLN:NE2	2.13	0.47
1:C:184:LYS:HE3	1:C:398:VAL:O	2.15	0.47
1:A:165:ARG:HD3	1:A:169:ASP:OD2	2.15	0.46
1:A:326:PRO:HA	1:A:327:GLY:HA3	1.70	0.46
1:B:335:VAL:H	1:D:200:GLN:NE2	2.13	0.46
1:B:426:ILE:HG23	1:B:430:ASN:HB2	1.97	0.46
1:A:99:PHE:HA	1:A:115:ASN:HD21	1.80	0.46
1:D:387:ALA:O	1:D:391:ILE:HG12	2.15	0.46
1:C:303:ASN:ND2	1:C:306:ARG:HH21	2.08	0.46
1:B:30:ARG:HG3	1:B:32:TRP:CH2	2.50	0.46
1:A:328:SER:HB2	1:A:334:LYS:CB	2.46	0.46
1:C:158:MSE:HG2	1:C:376:ALA:HB2	1.98	0.46
1:D:427:GLY:O	1:D:428:TYR:CB	2.64	0.46
1:D:434:ILE:HG23	1:D:448:GLU:HB2	1.98	0.46
1:A:184:LYS:HE3	1:A:401:ILE:O	2.16	0.46
1:A:227:MSE:HG2	1:B:227:MSE:SE	2.66	0.45
1:B:345:GLN:NE2	1:C:373:PRO:HD2	2.27	0.45
1:C:63:GLN:HE21	1:C:263:ILE:CD1	2.30	0.45
1:D:188:PHE:HB3	1:D:207:LEU:HB3	1.98	0.45
1:A:246:LEU:O	1:A:247:ASN:HB2	2.15	0.45
1:D:427:GLY:O	1:D:428:TYR:HB3	2.16	0.45
1:B:455:VAL:HG22	1:B:459:GLU:CB	2.41	0.45
1:C:61:VAL:HG11	1:C:153:THR:HG23	1.98	0.45
1:B:188:PHE:HB3	1:B:207:LEU:HB3	1.98	0.44
1:B:30:ARG:HD2	1:B:30:ARG:HA	1.68	0.44
1:D:184:LYS:HE3	1:D:401:ILE:O	2.17	0.44
1:D:414:ARG:O	1:D:414:ARG:HG3	2.17	0.44
1:A:372:ASN:HB2	1:A:373:PRO:HD3	1.98	0.44
1:D:151:ASN:O	1:D:278:LEU:HD22	2.18	0.44
1:B:255:LYS:HE3	1:B:259:GLU:OE2	2.17	0.44
1:A:303:ASN:ND2	1:A:306:ARG:HH21	2.07	0.44
1:D:113:ASN:HD21	1:D:145:ASN:HD21	1.65	0.44
1:A:335:VAL:H	1:C:200:GLN:NE2	2.15	0.44
1:A:335:VAL:H	1:C:200:GLN:HE21	1.66	0.43
1:C:30:ARG:HD3	1:C:30:ARG:HA	1.75	0.43
1:B:303:ASN:ND2	1:B:306:ARG:HE	2.17	0.43
1:B:426:ILE:HG23	1:B:430:ASN:CB	2.49	0.43
1:D:158:MSE:HG2	1:D:376:ALA:HB2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:338:THR:HG22	1:C:106:THR:HG22	2.00	0.43
1:A:188:PHE:HB3	1:A:207:LEU:HB3	2.00	0.43
1:D:372:ASN:HB2	1:D:373:PRO:HD3	1.99	0.42
1:D:392:SER:O	1:D:396:ASN:HB2	2.19	0.42
1:C:146:MSE:O	1:C:147:SER:HB2	2.19	0.42
1:A:430:ASN:O	1:A:434:ILE:HG12	2.19	0.42
1:B:303:ASN:HD22	1:B:306:ARG:NH2	2.01	0.42
1:A:426:ILE:HG22	1:A:426:ILE:O	2.18	0.42
1:B:430:ASN:O	1:B:434:ILE:HG12	2.20	0.42
1:B:467:GLU:H	1:B:467:GLU:CD	2.21	0.42
1:C:227:MSE:SE	1:D:227:MSE:HG2	2.69	0.42
1:A:106:THR:HG21	1:A:111:GLN:OE1	2.20	0.42
1:D:428:TYR:CG	1:D:429:ASP:N	2.88	0.42
1:D:330:ILE:H	1:D:330:ILE:HG13	1.69	0.41
1:A:473:ALA:HB3	1:B:247:ASN:H	1.86	0.41
1:A:30:ARG:HD3	1:A:30:ARG:HA	1.86	0.41
1:C:323:GLU:HG3	1:C:335:VAL:HG13	2.03	0.41
1:A:419:VAL:HG13	1:A:445:LEU:CD2	2.49	0.41
1:A:117:ASN:HD21	1:A:145:ASN:ND2	2.18	0.41
1:A:373:PRO:HD2	1:D:345:GLN:NE2	2.33	0.41
1:A:323:GLU:HG2	1:A:335:VAL:HG22	2.02	0.41
1:D:40:LEU:HD21	1:D:100:PRO:HB2	2.03	0.41
1:D:15:ARG:HD2	1:D:132:MSE:O	2.20	0.41
1:A:426:ILE:HG22	1:A:430:ASN:CB	2.49	0.41
1:A:15:ARG:HD2	1:A:132:MSE:O	2.20	0.41
1:D:312:PRO:HG3	1:D:333:GLY:CA	2.42	0.41
1:C:302:ALA:HB2	1:C:343:LEU:HD23	2.01	0.41
1:C:353:ASN:CG	1:C:378:ASN:HD22	2.24	0.41
1:D:291:ILE:HG23	1:D:386:LEU:HD12	2.03	0.41
1:A:435:ALA:CB	1:C:332:PRO:HG2	2.51	0.41
1:D:303:ASN:HD22	1:D:306:ARG:NH2	2.10	0.40
1:A:106:THR:HG22	1:D:338:THR:CG2	2.52	0.40
1:C:300:LYS:NZ	1:C:304:ASP:OD2	2.50	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	452/495 (91%)	437 (97%)	14 (3%)	1 (0%)	56	57
1	B	449/495 (91%)	440 (98%)	9 (2%)	0	100	100
1	C	405/495 (82%)	393 (97%)	12 (3%)	0	100	100
1	D	450/495 (91%)	437 (97%)	12 (3%)	1 (0%)	56	57
All	All	1756/1980 (89%)	1707 (97%)	47 (3%)	2 (0%)	59	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	428	TYR
1	A	335	VAL

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	350/372 (94%)	342 (98%)	8 (2%)	63	66
1	B	352/372 (95%)	346 (98%)	6 (2%)	73	78
1	C	319/372 (86%)	318 (100%)	1 (0%)	96	98
1	D	350/372 (94%)	343 (98%)	7 (2%)	68	72
All	All	1371/1488 (92%)	1349 (98%)	22 (2%)	75	79

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

Mol	Chain	Res	Type
1	A	74	ARG
1	A	189	ASP
1	A	325	GLU
1	A	328	SER
1	A	419	VAL
1	A	420	THR
1	A	425	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	455	VAL
1	B	30	ARG
1	B	149	SER
1	B	179	LYS
1	B	287	SER
1	B	325	GLU
1	B	426	ILE
1	C	189	ASP
1	D	18	THR
1	D	223	LYS
1	D	255	LYS
1	D	328	SER
1	D	455	VAL
1	D	458	GLU
1	D	467	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	69	ASN
1	A	105	GLN
1	A	115	ASN
1	A	143	HIS
1	A	145	ASN
1	A	148	GLN
1	A	200	GLN
1	A	292	ASN
1	A	303	ASN
1	A	339	GLN
1	A	345	GLN
1	A	349	GLN
1	A	378	ASN
1	A	396	ASN
1	B	63	GLN
1	B	98	HIS
1	B	105	GLN
1	B	115	ASN
1	B	145	ASN
1	B	148	GLN
1	B	200	GLN
1	B	292	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	303	ASN
1	B	339	GLN
1	B	345	GLN
1	B	349	GLN
1	B	378	ASN
1	B	396	ASN
1	C	63	GLN
1	C	69	ASN
1	C	98	HIS
1	C	105	GLN
1	C	115	ASN
1	C	145	ASN
1	C	148	GLN
1	C	247	ASN
1	C	292	ASN
1	C	303	ASN
1	C	339	GLN
1	C	345	GLN
1	C	349	GLN
1	C	378	ASN
1	C	396	ASN
1	D	35	GLN
1	D	63	GLN
1	D	69	ASN
1	D	105	GLN
1	D	115	ASN
1	D	145	ASN
1	D	148	GLN
1	D	200	GLN
1	D	247	ASN
1	D	292	ASN
1	D	303	ASN
1	D	339	GLN
1	D	345	GLN
1	D	349	GLN
1	D	378	ASN
1	D	396	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

3 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	C	501	-	4,4,4	0.20	0	6,6,6	0.29	0
2	SO4	D	501	-	4,4,4	0.19	0	6,6,6	0.12	0
2	SO4	D	502	-	4,4,4	0.16	0	6,6,6	0.08	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
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	502	-	-	0/0/0/0	0/0/0/0

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	456/495 (92%)	0.09	20 (4%) 33 37	12, 24, 51, 62	0
1	B	453/495 (91%)	-0.13	9 (1%) 62 67	12, 23, 44, 50	0
1	C	411/495 (83%)	-0.01	11 (2%) 52 57	11, 22, 42, 66	0
1	D	454/495 (91%)	0.11	25 (5%) 24 26	11, 24, 59, 73	0
All	All	1774/1980 (89%)	0.02	65 (3%) 39 44	11, 23, 49, 73	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	428	TYR	7.0
1	D	453	GLY	5.1
1	A	78	ALA	4.6
1	D	450	VAL	4.6
1	D	419	VAL	4.5
1	C	418	LEU	4.4
1	A	335	VAL	4.3
1	D	456	THR	4.2
1	D	458	GLU	4.2
1	B	472	PRO	4.0
1	A	451	GLY	3.7
1	D	455	VAL	3.6
1	C	472	PRO	3.5
1	A	473	ALA	3.5
1	D	463	VAL	3.5
1	D	460	PHE	3.4
1	B	326	PRO	3.3
1	A	454	TYR	3.3
1	D	440	LYS	3.3
1	D	457	ASP	3.3
1	B	335	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	359	PHE	3.2
1	C	416	LEU	3.2
1	C	413	ASP	3.1
1	A	440	LYS	3.0
1	D	359	PHE	3.0
1	A	450	VAL	2.9
1	A	426	ILE	2.8
1	B	429	ASP	2.8
1	C	21	PHE	2.7
1	D	437	THR	2.7
1	A	452	GLY	2.7
1	B	359	PHE	2.7
1	C	350	VAL	2.6
1	A	328	SER	2.6
1	D	443	THR	2.6
1	C	333	GLY	2.5
1	D	454	TYR	2.5
1	D	433	LYS	2.5
1	B	356	ALA	2.5
1	A	425	LYS	2.4
1	C	410	ALA	2.4
1	A	430	ASN	2.4
1	A	423	ALA	2.4
1	D	449	ALA	2.4
1	D	414	ARG	2.3
1	D	413	ASP	2.3
1	A	453	GLY	2.3
1	C	327	GLY	2.2
1	A	359	PHE	2.2
1	D	434	ILE	2.2
1	D	429	ASP	2.2
1	A	441	ASN	2.1
1	B	419	VAL	2.1
1	A	424	PRO	2.1
1	A	438	ALA	2.1
1	A	334	LYS	2.1
1	C	332	PRO	2.1
1	A	150	SER	2.1
1	D	358	THR	2.1
1	D	461	ASP	2.1
1	B	357	LEU	2.0
1	D	442	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	355	ALA	2.0
1	D	333	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	D	501	5/5	0.20	7.20	71,71,71,71	0
2	SO4	C	501	5/5	0.17	0.79	65,65,66,66	0
2	SO4	D	502	5/5	0.16	0.54	83,84,84,84	0

6.5 Other polymers ⓘ

There are no such residues in this entry.