



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:55 AM UTC

PDB ID : 4HGV / pdb_00004hgv
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 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

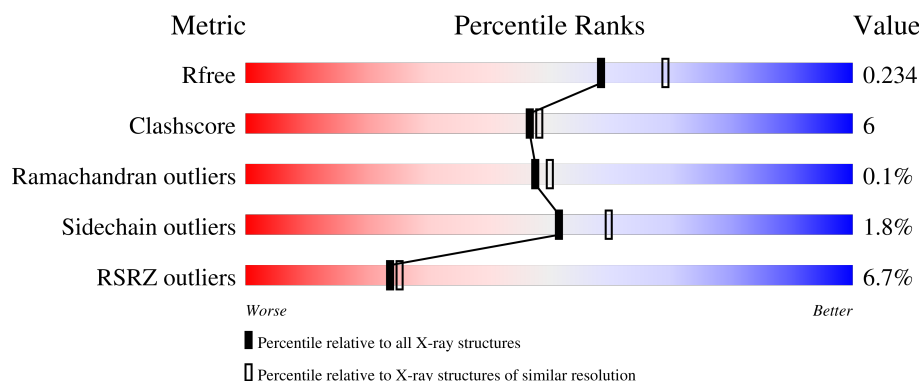
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	495	5% 80% 12% • 8%
1	B	495	3% 82% 9% • 8%
1	C	495	4% 74% 9% 17%
1	D	495	11% 79% 12% 8%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13548 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 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 (CCD ID: 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		

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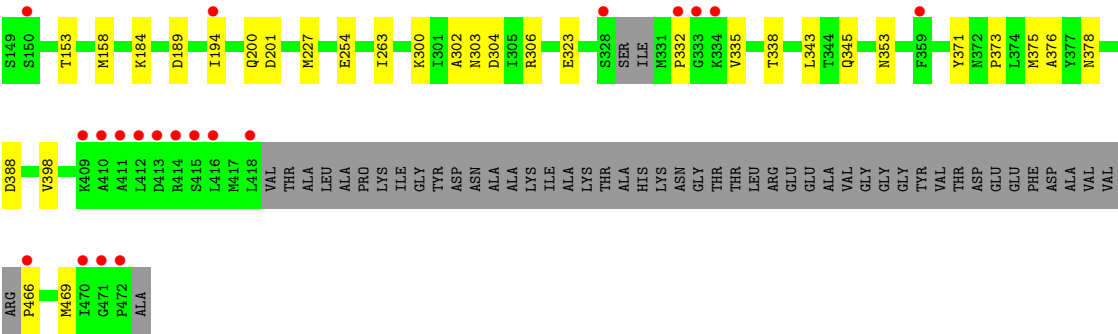
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

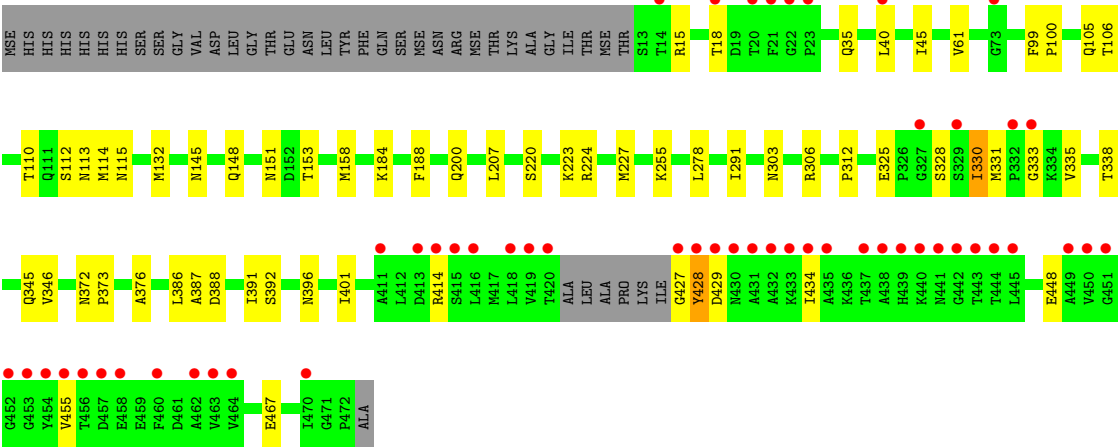
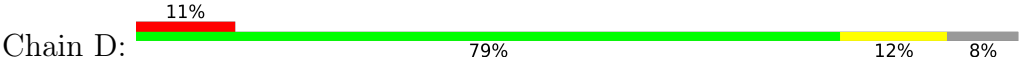
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	82	Total	O	0	0
			82	82		
3	C	77	Total	O	0	0
			77	77		
3	D	80	Total	O	0	0
			80	80		

- Molecule 1: Fumarate hydratase class II





● 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) 99.0 (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 0.198 , 0.234	Depositor DCC
R_{free} test set	5509 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.003 for -h,l,k	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.

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: 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	0.64	0/3439	0.86	0/4653
1	B	0.66	0/3440	0.88	2/4652 (0.0%)
1	C	0.66	0/3107	0.86	0/4199
1	D	0.67	0/3432	0.87	2/4640 (0.0%)
All	All	0.66	0/13418	0.87	4/18144 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	SER	CA-C-N	5.09	127.62	120.28
1	B	28	SER	C-N-CA	5.09	127.62	120.28
1	D	325	GLU	CA-C-N	5.03	125.31	119.93
1	D	325	GLU	C-N-CA	5.03	125.31	119.93

There are no chirality outliers.

There are no planarity outliers.

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	3388	0	3352	54	0
1	B	3388	0	3368	42	0
1	C	3060	0	3031	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	C	77	0	0	1	0
3	D	80	0	0	1	0
All	All	13548	0	13092	149	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 6.

All (149) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:29:ASP:HB3	1:B:30:ARG:HD3	1.80	0.62
1:B:105:GLN:HE22	1:B:112:SER:H	1.47	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
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:31:TYR:H	1:B:98:HIS:CD2	2.23	0.56
1:B:428:TYR:CE1	1:D:330:ILE:HG12	2.40	0.56
1:D:303:ASN:ND2	1:D:306:ARG:HE	2.04	0.56
1:A:61:VAL:HG11	1:A:153:THR:HG23	1.88	0.55
1:C:105:GLN:HE22	1:C:112:SER:H	1.52	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:31:TYR:H	1:C:98:HIS:HD2	1.55	0.51
1:C:466:PRO:CA	1:C:469:MSE:HE3	2.33	0.51
1:D:220:SER:O	1:D:224:ARG:HG3	2.10	0.51
1:D:303:ASN:ND2	1:D:306:ARG:HH21	2.05	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:A:45:ILE:HA	1:D:388:ASP:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:MSE:HG2	1:D:227:MSE:SE	2.62	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
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:467:GLU:H	1:B:467:GLU:CD	2.21	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:A:328:SER:HB2	1:A:334:LYS:CB	2.46	0.46
1:B:30:ARG:HG3	1:B:32:TRP:CH2	2.50	0.46
1:C:158:MSE:HG2	1:C:376:ALA:HB2	1.98	0.46
1:C:303:ASN:ND2	1:C:306:ARG:HH21	2.08	0.46
1:D:427:GLY:O	1:D:428:TYR:CB	2.64	0.46
1:A:184:LYS:HE3	1:A:401:ILE:O	2.16	0.46
1:D:434:ILE:HG23	1:D:448:GLU:HB2	1.98	0.46
1:A:227:MSE:HG2	1:B:227:MSE:SE	2.66	0.45
1:C:353:ASN:CG	1:C:378:ASN:HD22	2.24	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:C:300:LYS:NZ	1:C:304:ASP:OD2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:335:VAL:H	1:C:200:GLN:NE2	2.15	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:HE21	1.66	0.43
1:C:30:ARG:HA	1:C:30:ARG:HD3	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
1:A:188:PHE:HB3	1:A:207:LEU:HB3	2.00	0.43
1:B:338:THR:HG22	1:C:106:THR:HG22	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:A:426:ILE:HG22	1:A:426:ILE:O	2.18	0.42
1:B:303:ASN:HD22	1:B:306:ARG:NH2	2.01	0.42
1:B:430:ASN:O	1:B:434:ILE:HG12	2.20	0.42
1:A:106:THR:HG21	1:A:111:GLN:OE1	2.20	0.42
1:C:227:MSE:SE	1:D:227:MSE:HG2	2.69	0.42
1:D:428:TYR:CG	1:D:429:ASP:N	2.88	0.42
1:A:30:ARG:HD3	1:A:30:ARG:HA	1.86	0.41
1:A:473:ALA:HB3	1:B:247:ASN:H	1.86	0.41
1:D:330:ILE:H	1:D:330:ILE:HG13	1.69	0.41
1:C:323:GLU:HG3	1:C:335:VAL:HG13	2.03	0.41
1:A:117:ASN:HD21	1:A:145:ASN:ND2	2.18	0.41
1:A:419:VAL:HG13	1:A:445:LEU:CD2	2.49	0.41
1:A:323:GLU:HG2	1:A:335:VAL:HG22	2.02	0.41
1:A:373:PRO:HD2	1:D:345:GLN:NE2	2.33	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:15:ARG:HD2	1:A:132:MSE:O	2.20	0.41
1:A:426:ILE:HG22	1:A:430:ASN:CB	2.49	0.41
1:C:302:ALA:HB2	1:C:343:LEU:HD23	2.01	0.41
1:D:312:PRO:HG3	1:D:333:GLY:CA	2.42	0.41
1:A:435:ALA:CB	1:C:332:PRO:HG2	2.51	0.41
1:D:291:ILE:HG23	1:D:386:LEU:HD12	2.03	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

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	452/495 (91%)	437 (97%)	14 (3%)	1 (0%)	43	44
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%)	43	44
All	All	1756/1980 (89%)	1707 (97%)	47 (3%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

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

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	350/372 (94%)	341 (97%)	9 (3%)	40	46
1	B	352/372 (95%)	346 (98%)	6 (2%)	53	62
1	C	319/372 (86%)	318 (100%)	1 (0%)	86	91
1	D	350/372 (94%)	342 (98%)	8 (2%)	44	51
All	All	1371/1488 (92%)	1347 (98%)	24 (2%)	51	60

All (24) 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	346	VAL
1	A	419	VAL
1	A	420	THR
1	A	425	LYS
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	330	ILE
1	D	346	VAL
1	D	455	VAL
1	D	467	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
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	159	HIS
1	A	190	HIS
1	A	247	ASN
1	A	281	HIS
1	A	292	ASN
1	A	303	ASN
1	A	339	GLN

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Mol	Chain	Res	Type
1	A	345	GLN
1	A	349	GLN
1	A	378	ASN
1	A	396	ASN
1	B	98	HIS
1	B	105	GLN
1	B	115	ASN
1	B	145	ASN
1	B	148	GLN
1	B	190	HIS
1	B	200	GLN
1	B	292	ASN
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	200	GLN
1	C	247	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	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	303	ASN

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Mol	Chain	Res	Type
1	D	324	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 [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](#)

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	D	502	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	C	501	-	4,4,4	0.29	0	6,6,6	0.29	0
2	SO4	D	501	-	4,4,4	0.25	0	6,6,6	0.13	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.

No monomer is involved in short contacts.

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	446/495 (90%)	0.19	25 (5%) 30 32	12, 24, 51, 62	0
1	B	443/495 (89%)	0.04	16 (3%) 46 48	12, 23, 44, 50	0
1	C	400/495 (80%)	-0.00	22 (5%) 30 32	11, 22, 40, 63	0
1	D	443/495 (89%)	0.31	53 (11%) 9 9	11, 23, 59, 73	0
All	All	1732/1980 (87%)	0.14	116 (6%) 24 25	11, 23, 49, 73	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	428	TYR	7.5
1	D	427	GLY	5.9
1	D	419	VAL	5.7
1	C	416	LEU	5.5
1	A	473	ALA	5.3
1	A	428	TYR	4.9
1	D	450	VAL	4.5
1	D	420	THR	4.5
1	A	335	VAL	4.5
1	C	418	LEU	4.5
1	D	455	VAL	4.4
1	D	463	VAL	4.4
1	C	472	PRO	4.4
1	D	431	ALA	4.3
1	C	332	PRO	4.3
1	D	445	LEU	4.2
1	C	21	PHE	4.2
1	D	418	LEU	4.2
1	D	434	ILE	4.0
1	B	326	PRO	4.0
1	D	429	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	449	ALA	3.9
1	D	432	ALA	3.7
1	D	333	GLY	3.7
1	B	472	PRO	3.7
1	A	150	SER	3.7
1	D	456	THR	3.6
1	C	333	GLY	3.6
1	D	454	TYR	3.6
1	A	426	ILE	3.5
1	C	412	LEU	3.5
1	D	433	LYS	3.5
1	C	411	ALA	3.4
1	B	419	VAL	3.4
1	D	416	LEU	3.3
1	D	437	THR	3.3
1	A	327	GLY	3.3
1	B	426	ILE	3.3
1	D	435	ALA	3.2
1	A	334	LYS	3.2
1	C	470	ILE	3.2
1	D	458	GLU	3.2
1	D	451	GLY	3.2
1	D	20	THR	3.1
1	C	466	PRO	3.1
1	D	14	THR	3.0
1	D	452	GLY	3.0
1	D	414	ARG	2.9
1	B	335	VAL	2.8
1	D	443	THR	2.8
1	D	329	SER	2.8
1	D	438	ALA	2.8
1	D	444	THR	2.8
1	C	413	ASP	2.8
1	A	326	PRO	2.8
1	D	442	GLY	2.7
1	D	460	PHE	2.7
1	D	457	ASP	2.7
1	C	20	THR	2.7
1	B	428	TYR	2.7
1	D	430	ASN	2.7
1	C	471	GLY	2.7
1	A	435	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	430	ASN	2.7
1	D	464	VAL	2.7
1	D	413	ASP	2.7
1	D	22	GLY	2.6
1	A	432	ALA	2.6
1	A	424	PRO	2.6
1	D	21	PHE	2.6
1	B	429	ASP	2.6
1	D	439	HIS	2.6
1	D	440	LYS	2.6
1	A	78	ALA	2.6
1	A	328	SER	2.6
1	C	359	PHE	2.5
1	A	440	LYS	2.5
1	C	334	LYS	2.5
1	C	194	ILE	2.5
1	C	415	SER	2.4
1	A	425	LYS	2.4
1	D	415	SER	2.4
1	D	453	GLY	2.4
1	A	359	PHE	2.3
1	C	410	ALA	2.3
1	B	471	GLY	2.3
1	B	29	ASP	2.3
1	C	409	LYS	2.3
1	A	430	ASN	2.3
1	D	462	ALA	2.3
1	A	454	TYR	2.3
1	B	422	LEU	2.3
1	D	470	ILE	2.3
1	A	431	ALA	2.3
1	D	327	GLY	2.3
1	C	150	SER	2.2
1	A	406	ASP	2.2
1	B	423	ALA	2.2
1	A	416	LEU	2.2
1	D	18	THR	2.2
1	A	442	GLY	2.1
1	D	73	GLY	2.1
1	A	438	ALA	2.1
1	D	441	ASN	2.1
1	D	332	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	427	GLY	2.1
1	D	411	ALA	2.1
1	C	328	SER	2.1
1	A	420	THR	2.1
1	B	150	SER	2.1
1	D	40	LEU	2.1
1	C	414	ARG	2.1
1	D	23	PRO	2.1
1	B	452	GLY	2.1
1	B	323	GLU	2.0
1	B	420	THR	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
2	SO4	D	501	5/5	0.71	0.18	71,71,71,71	0
2	SO4	C	501	5/5	0.74	0.17	65,65,66,66	0
2	SO4	D	502	5/5	0.74	0.19	83,84,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.