Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:11 PM GMT

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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 (NYSGRC)
Deposited on	:	2012-10-08
Resolution	:	2.09 Å(reported)

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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	Percentile Ranks	Value
Rfree		0.234
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		1.6%
RSRZ outliers		5.6%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
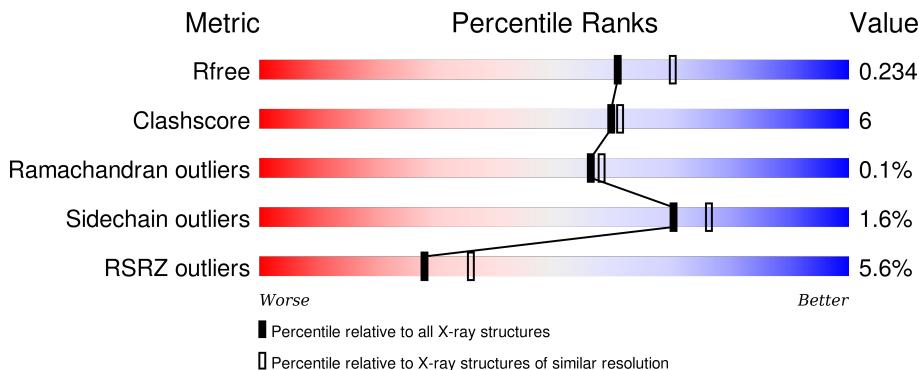
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	495	6% / 80% 12% · 8%
1	B	495	2% / 82% 9% · 8%
1	C	495	4% / 74% 9% 17%
1	D	495	7% / 79% 12% 8%
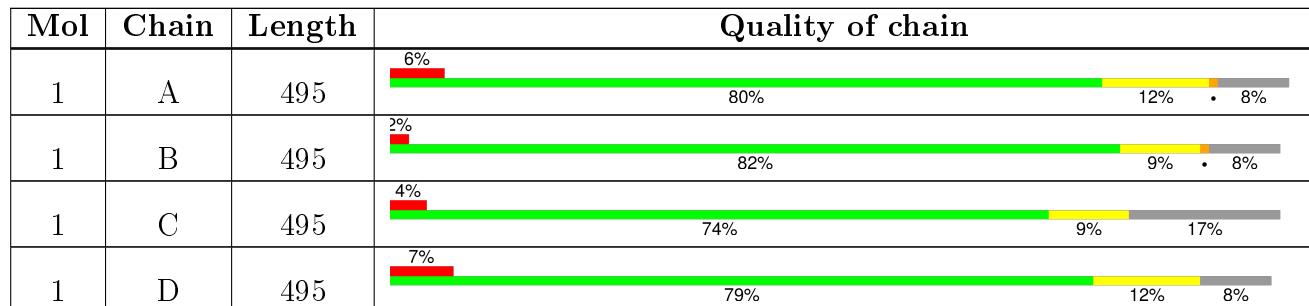
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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
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 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 3388	C 2124	N 596	O 653	S 5	Se 10	0	0	0
1	B	453	Total 3388	C 2128	N 595	O 650	S 5	Se 10	0	0	0
1	C	411	Total 3060	C 1923	N 536	O 586	S 5	Se 10	0	0	0
1	D	454	Total 3381	C 2121	N 593	O 651	S 5	Se 11	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
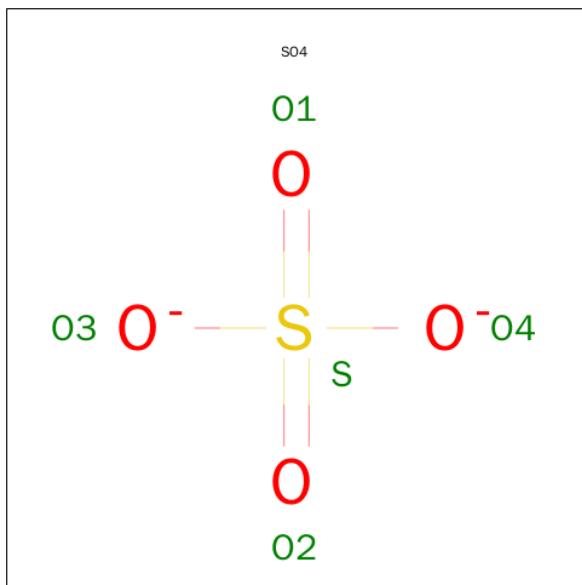
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 5	O 4	S 1	0	0
2	D	1	Total 5	O 4	S 1	0	0

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

- Molecule 3 is water.

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

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
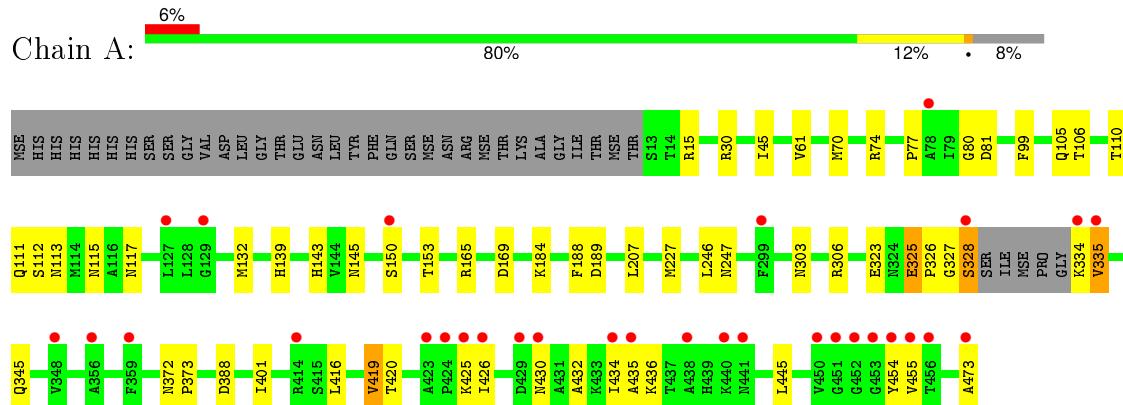
- Molecule 1: Fumarate hydratase class II

- Molecule 1: Fumarate hydratase class II

- Molecule 1: Fumarate hydratase class II

Chain D:
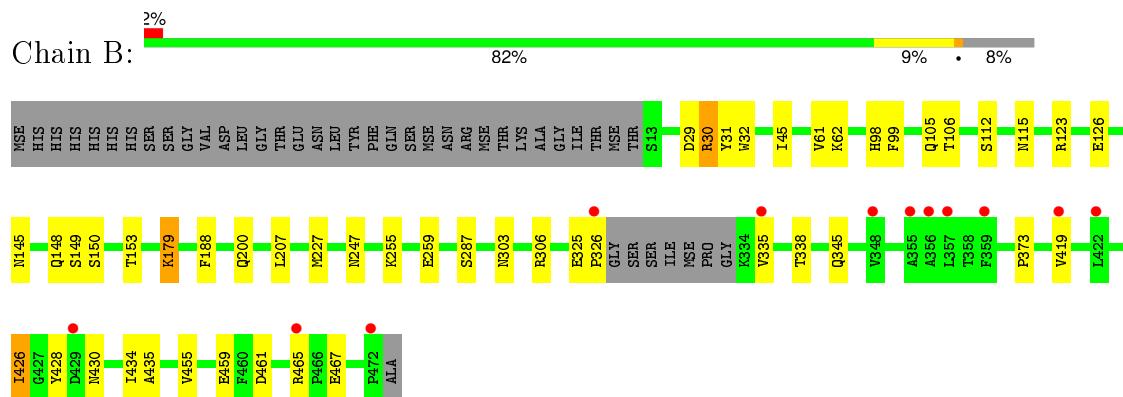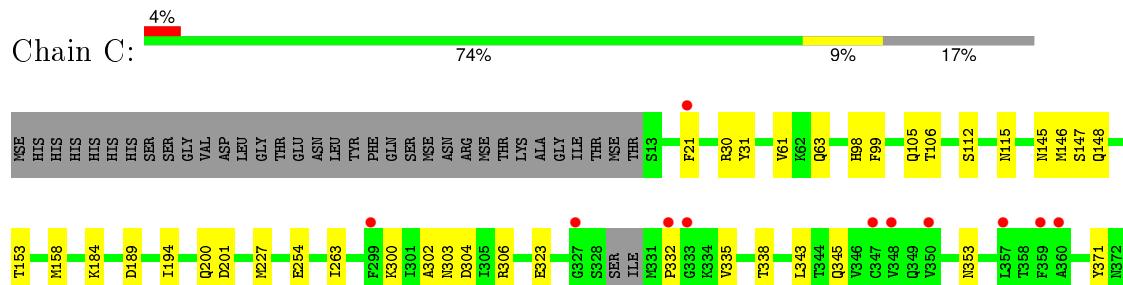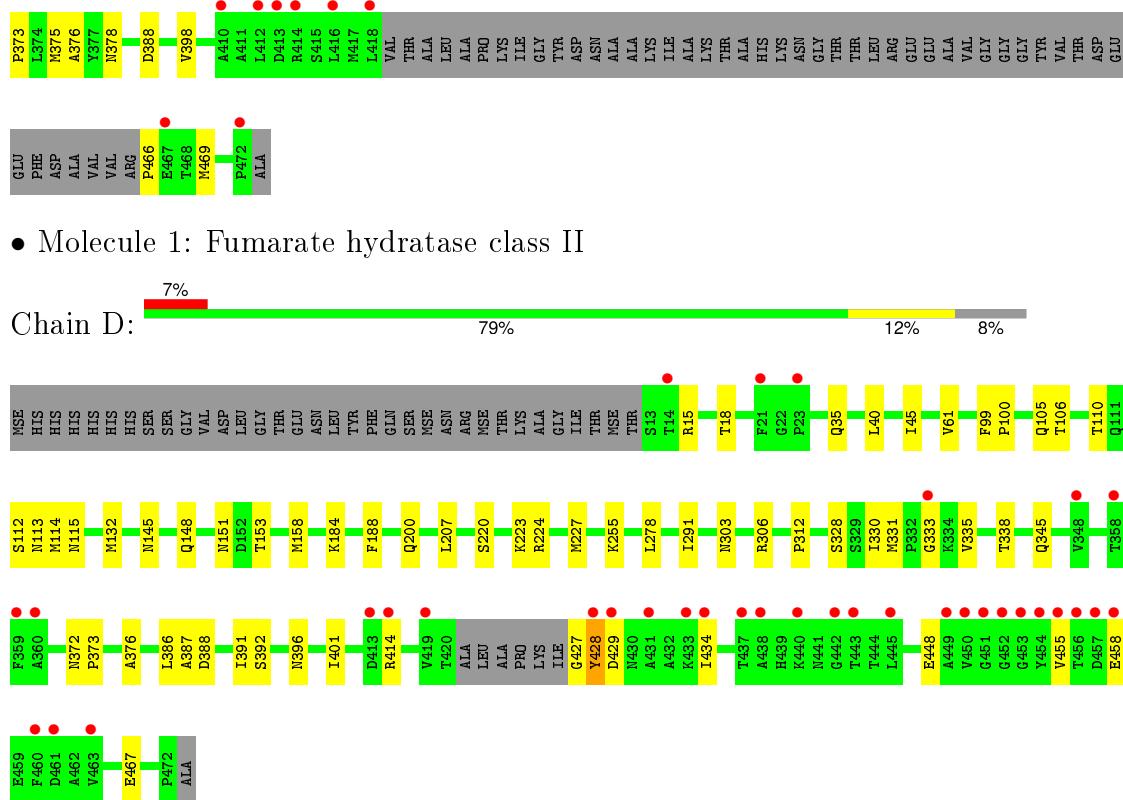
4　Data and refinement statistics (i)

| 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
$< I/\sigma(I) >$ [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 (5.27%)	DCC
Wilson B-factor (Å^2)	22.7	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.4	EDS
Estimated twinning fraction	0.003 for -h,l,k	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	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.*

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[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 (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	0.50	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 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	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
3	C	77	0	0	1	0

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 (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%)	52	53
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%)	52	53
All	All	1756/1980 (89%)	1707 (97%)	47 (3%)	2 (0%)	56	58

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%)	342 (98%)	8 (2%)	58	62
1	B	352/372 (95%)	346 (98%)	6 (2%)	68	74
1	C	319/372 (86%)	318 (100%)	1 (0%)	94	97
1	D	350/372 (94%)	343 (98%)	7 (2%)	63	68
All	All	1371/1488 (92%)	1349 (98%)	22 (2%)	70	76

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
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

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Mol	Chain	Res	Type
1	B	105	GLN
1	B	115	ASN
1	B	145	ASN
1	B	148	GLN
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	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

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Mol	Chain	Res	Type
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 carbohydrates 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	C	501	-	4,4,4	0.20	0	6,6,6	0.31	0
2	SO4	D	501	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	D	502	-	4,4,4	0.18	0	6,6,6	0.09	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.18	31 (6%)	19	26	12, 24, 51, 62	0
1	B	443/495 (89%)	-0.08	12 (2%)	58	65	12, 23, 44, 50	0
1	C	400/495 (80%)	0.05	19 (4%)	34	43	11, 22, 40, 63	0
1	D	443/495 (89%)	0.22	35 (7%)	15	21	11, 23, 59, 73	0
All	All	1732/1980 (87%)	0.09	97 (5%)	28	36	11, 23, 49, 73	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	428	TYR	8.2
1	D	450	VAL	6.1
1	D	453	GLY	5.9
1	D	419	VAL	5.0
1	C	418	LEU	4.9
1	D	458	GLU	4.9
1	D	456	THR	4.9
1	A	78	ALA	4.6
1	A	335	VAL	4.5
1	C	472	PRO	4.5
1	A	451	GLY	4.4
1	D	455	VAL	4.4
1	B	472	PRO	4.4
1	D	463	VAL	4.3
1	D	460	PHE	4.1
1	A	473	ALA	3.9
1	D	440	LYS	3.9
1	C	359	PHE	3.8
1	C	416	LEU	3.7
1	C	413	ASP	3.5
1	D	457	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	359	PHE	3.5
1	B	326	PRO	3.4
1	D	443	THR	3.4
1	B	335	VAL	3.4
1	C	21	PHE	3.3
1	A	454	TYR	3.3
1	A	450	VAL	3.3
1	A	426	ILE	3.2
1	A	440	LYS	3.2
1	B	359	PHE	3.1
1	A	430	ASN	3.1
1	A	452	GLY	3.1
1	D	433	LYS	3.1
1	B	429	ASP	3.0
1	D	449	ALA	3.0
1	A	424	PRO	3.0
1	D	414	ARG	2.9
1	D	442	GLY	2.9
1	B	356	ALA	2.9
1	A	453	GLY	2.9
1	B	419	VAL	2.9
1	D	454	TYR	2.9
1	C	327	GLY	2.8
1	C	350	VAL	2.8
1	C	333	GLY	2.8
1	D	434	ILE	2.7
1	A	425	LYS	2.7
1	A	328	SER	2.7
1	A	423	ALA	2.7
1	D	438	ALA	2.7
1	D	461	ASP	2.6
1	D	437	THR	2.6
1	C	348	VAL	2.6
1	A	359	PHE	2.6
1	A	438	ALA	2.6
1	D	413	ASP	2.5
1	D	358	THR	2.5
1	A	334	LYS	2.4
1	C	299	PHE	2.4
1	A	435	ALA	2.4
1	C	467	GLU	2.4
1	A	356	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	431	ALA	2.3
1	D	451	GLY	2.3
1	A	441	ASN	2.3
1	B	357	LEU	2.3
1	A	299	PHE	2.3
1	D	348	VAL	2.3
1	D	429	ASP	2.3
1	D	452	GLY	2.3
1	C	347	CYS	2.3
1	C	332	PRO	2.3
1	C	357	LEU	2.3
1	D	14	THR	2.2
1	D	333	GLY	2.2
1	B	355	ALA	2.2
1	B	465	ARG	2.2
1	C	410	ALA	2.2
1	A	456	THR	2.2
1	D	23	PRO	2.2
1	A	414	ARG	2.1
1	A	127	LEU	2.1
1	A	348	VAL	2.1
1	D	21	PHE	2.1
1	C	414	ARG	2.1
1	A	434	ILE	2.1
1	B	422	LEU	2.1
1	D	445	LEU	2.1
1	C	360	ALA	2.1
1	D	360	ALA	2.1
1	B	348	VAL	2.1
1	C	412	LEU	2.1
1	A	150	SER	2.0
1	A	429	ASP	2.0
1	A	129	GLY	2.0
1	A	455	VAL	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 (i)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	D	501	5/5	0.88	0.21	6.92	71,71,71,71	0
2	SO4	C	501	5/5	0.88	0.18	0.92	65,65,66,66	0
2	SO4	D	502	5/5	0.91	0.17	0.73	83,84,84,84	0

6.5 Other polymers (i)

There are no such residues in this entry.