



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:21 am GMT

PDB ID : 4RX4
Title : Crystal structure of VH1-46 germline-derived CD4-binding site-directed anti-body 8ANC134 in complex with HIV-1 clade A Q842.d12 gp120
Authors : Zhou, T.; Acharya, P.; Moquin, S.; Kwong, P.D.
Deposited on : 2014-12-08
Resolution : 3.45 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

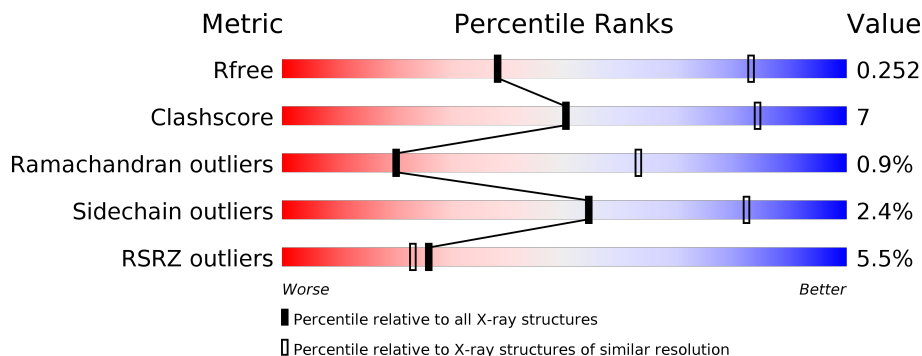
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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}	100719	1135 (3.56-3.36)
Clashscore	112137	1040 (3.52-3.40)
Ramachandran outliers	110173	1009 (3.52-3.40)
Sidechain outliers	110143	1010 (3.52-3.40)
RSRZ outliers	101464	1017 (3.54-3.38)

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 $\leq 5\%$. 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	E	354	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>10%</div> </div> </div>
1	G	354	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>8%</div> </div> </div>
2	A	229	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>• •</div> </div> </div>
2	H	229	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>5%</div> </div> </div>
3	D	213	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>13%</div> </div> </div>
3	L	213	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>•</div> </div> </div>

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
4	NAG	E	501	-	-	-	X
4	NAG	E	502	-	-	-	X
4	NAG	E	503	-	-	-	X
4	NAG	G	504	-	-	-	X
4	NAG	G	505	-	-	-	X
5	SO4	A	301	-	-	-	X
5	SO4	D	302	-	-	-	X
5	SO4	D	304	-	-	-	X
5	SO4	G	512	-	-	-	X
5	SO4	L	403	-	-	-	X
6	EDO	E	507	-	-	-	X
6	EDO	G	509	-	-	-	X
6	EDO	G	513	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 23562 atoms, of which 11587 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 HIV-1 Clade A Q842.d12 gp120.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	325	Total	C	H	N	O	S	0	0	0
			5094	1627	2504	459	483	21			
1	E	320	Total	C	H	N	O	S	0	0	0
			5026	1606	2472	452	475	21			

- Molecule 2 is a protein called 8ANC134 Heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	217	Total	C	H	N	O	S	0	0	0
			3258	1038	1623	280	311	6			
2	A	222	Total	C	H	N	O	S	0	0	0
			3300	1060	1627	287	319	7			

- Molecule 3 is a protein called 8ANC134 Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	212	Total	C	H	N	O	S	0	0	0
			3226	1025	1586	285	325	5			
3	D	213	Total	C	H	N	O	S	0	0	0
			3240	1030	1591	286	328	5			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



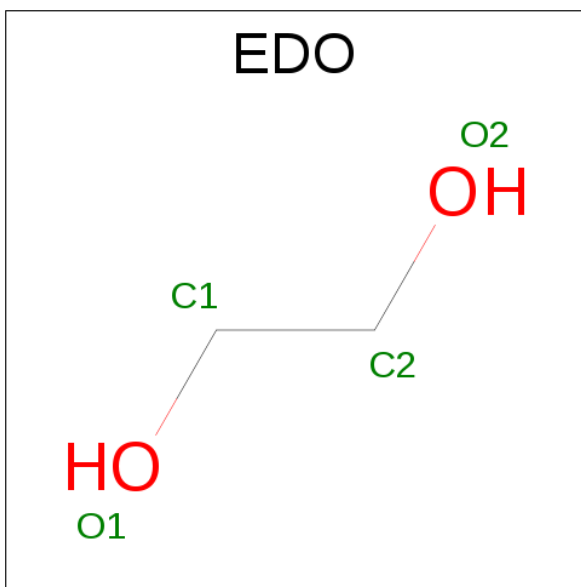
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	G	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		
4	E	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

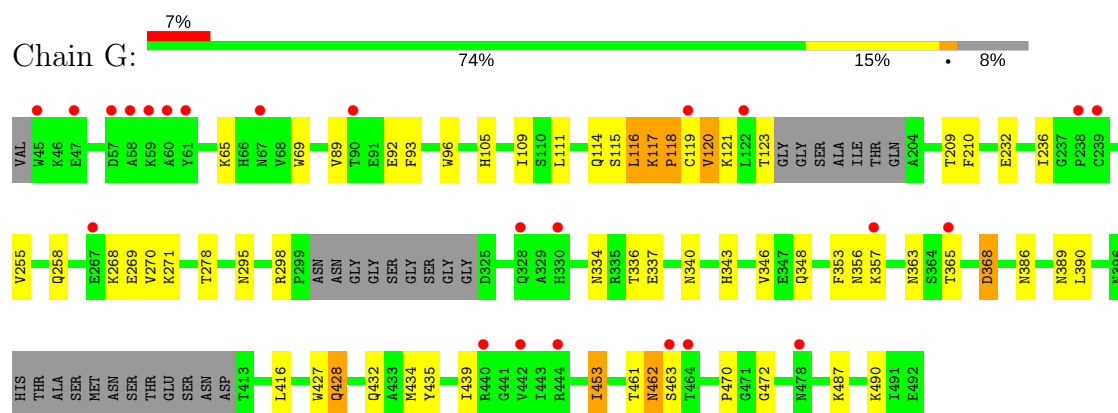


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	G	1	Total	C	H	O	0	0
			10	2	6	2		
6	E	1	Total	C	H	O	0	0
			10	2	6	2		

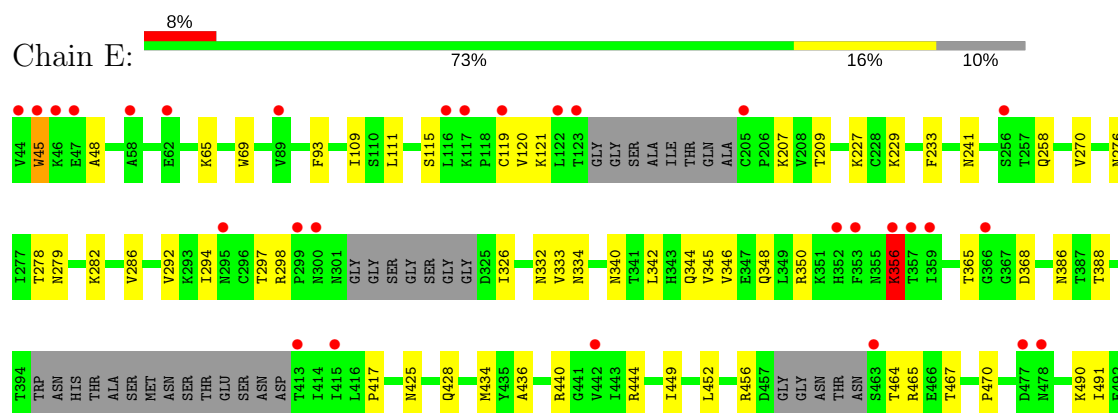
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

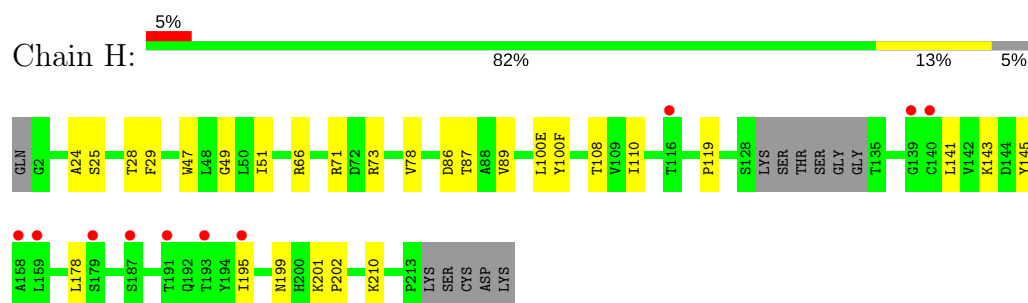
• Molecule 1: HIV-1 Clade A Q842.d12 gp120



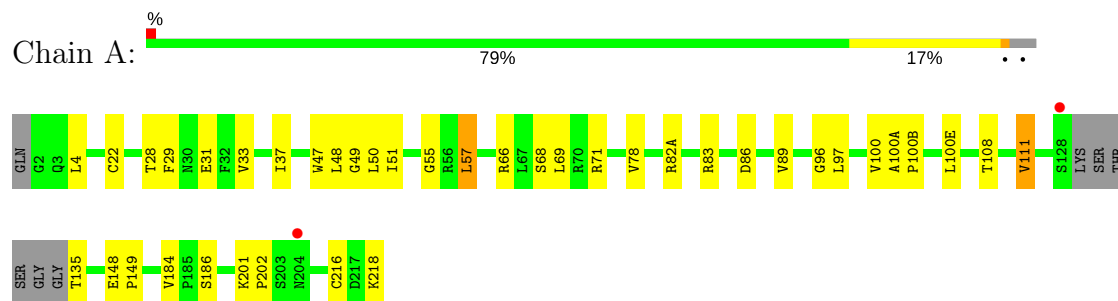
• Molecule 1: HIV-1 Clade A Q842.d12 gp120



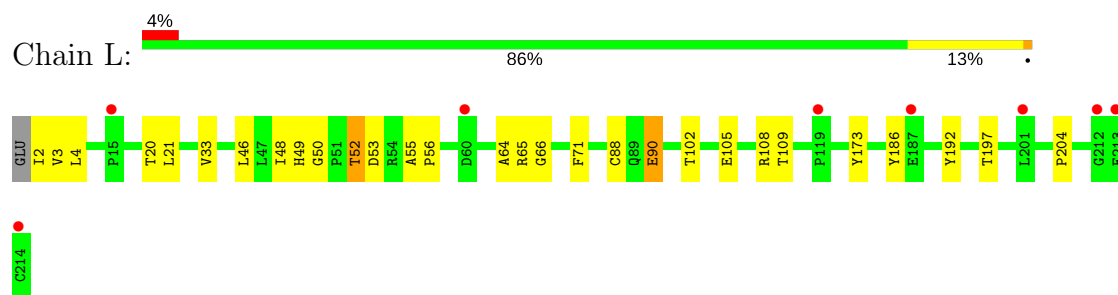
• Molecule 2: 8ANC134 Heavy chain



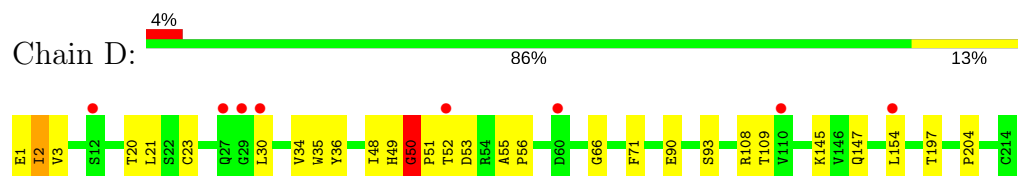
- Molecule 2: 8ANC134 Heavy chain



- Molecule 3: 8ANC134 Light Chain



- Molecule 3: 8ANC134 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	220.35Å 220.35Å 118.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.90 – 3.45 26.90 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (26.90-3.45) 93.2 (26.90-3.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.46Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1690)	Depositor
R, R_{free}	0.208 , 0.253 0.210 , 0.252	Depositor DCC
R_{free} test set	1406 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	99.8	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 98.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23562	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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

5.1 Standard geometry

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

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	E	0.41	0/2607	0.70	0/3535
1	G	0.44	0/2646	0.70	0/3590
2	A	0.41	0/1711	0.64	0/2326
2	H	0.42	0/1673	0.65	0/2277
3	D	0.39	0/1687	0.65	0/2291
3	L	0.40	0/1678	0.64	0/2279
All	All	0.41	0/12002	0.67	0/16298

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	E	0	1
3	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	50	GLY	Peptide
1	E	356	LYS	Peptide

5.2 Too-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 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	E	2554	2472	2505	38	0
1	G	2590	2504	2530	38	0
2	A	1673	1627	1667	23	0
2	H	1635	1623	1628	21	0
3	D	1649	1591	1597	17	0
3	L	1640	1586	1589	22	0
4	E	70	70	65	6	0
4	G	84	84	78	4	0
5	A	5	0	0	0	0
5	D	20	0	0	1	0
5	E	5	0	0	0	0
5	G	15	0	0	1	0
5	L	15	0	0	0	0
6	E	4	6	6	0	0
6	G	16	24	24	1	0
All	All	11975	11587	11689	156	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 7.

All (156) 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:E:241:ASN:ND2	4:E:504:NAG:O5	2.14	0.80
1:G:298:ARG:NH2	1:G:439:ILE:O	2.23	0.72
1:G:365:THR:HG21	6:G:513:EDO:H21	1.73	0.69
1:E:276:ASN:ND2	4:E:501:NAG:O7	2.25	0.69
1:G:353:PHE:HA	1:G:356:ASN:HB2	1.74	0.69
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.28	0.66
1:E:388:THR:OG1	4:E:503:NAG:O7	2.15	0.65
3:L:65:ARG:HG2	3:L:66:GLY:N	2.13	0.64
1:G:368:ASP:OD1	1:G:368:ASP:N	2.31	0.63
3:D:21:LEU:HD11	3:D:35:TRP:CZ3	2.35	0.62
2:A:68:SER:OG	2:A:82(A):ARG:NH2	2.32	0.61
1:G:334:ASN:HB3	1:G:337:GLU:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:ASP:OD2	1:E:425:ASN:ND2	2.35	0.60
1:E:278:THR:O	3:D:93:SER:OG	2.19	0.59
2:A:100(A):ALA:HB1	2:A:100(B):PRO:HD2	1.84	0.59
1:G:232:GLU:CB	1:G:271:LYS:HE2	2.34	0.58
1:E:227:LYS:HE2	1:E:229:LYS:HD3	1.86	0.57
1:G:363:ASN:ND2	4:G:504:NAG:O7	2.37	0.57
1:G:270:VAL:HG23	1:G:348:GLN:HG3	1.86	0.57
1:E:340:ASN:O	1:E:344:GLN:NE2	2.37	0.57
1:E:45:TRP:CD1	1:E:45:TRP:O	2.58	0.56
3:D:2:ILE:HD12	3:D:30:LEU:HD21	1.87	0.56
1:G:118:PRO:HG3	1:G:435:TYR:CE1	2.41	0.56
2:H:195:ILE:HG12	2:H:210:LYS:HB2	1.88	0.55
1:E:298:ARG:NH1	1:E:326:ILE:O	2.38	0.55
1:G:269:GLU:OE1	1:G:348:GLN:NE2	2.39	0.55
2:A:83:ARG:O	2:A:111:VAL:HG21	2.07	0.54
1:E:294:ILE:HD13	1:E:333:VAL:HB	1.88	0.54
3:L:197:THR:HG22	3:L:204:PRO:HG3	1.90	0.54
2:A:29:PHE:CZ	2:A:71:ARG:HD2	2.43	0.54
2:A:135:THR:N	2:A:186:SER:HG	2.07	0.53
1:G:120:VAL:HG13	1:G:121:LYS:HA	1.91	0.53
2:H:24:ALA:HB1	2:H:28:THR:HG23	1.89	0.52
1:G:120:VAL:CG1	1:G:121:LYS:HA	2.38	0.52
1:G:269:GLU:HG3	1:G:271:LYS:HE3	1.92	0.52
4:G:505:NAG:O3	4:G:505:NAG:O7	2.26	0.52
1:G:65:LYS:HB3	1:G:115:SER:HB2	1.92	0.52
3:D:66:GLY:HA3	3:D:71:PHE:HA	1.92	0.51
2:A:33:VAL:HG21	2:A:97:LEU:HD12	1.92	0.51
3:D:108:ARG:HG2	3:D:109:THR:N	2.26	0.51
4:G:506:NAG:O7	4:G:506:NAG:O3	2.25	0.50
1:G:109:ILE:HG12	1:G:428:GLN:HB3	1.93	0.50
1:E:342:LEU:O	1:E:345:VAL:HG22	2.11	0.50
1:E:456:ARG:NH1	5:D:301:SO4:O3	2.43	0.50
2:H:25:SER:OG	2:H:28:THR:HG22	2.12	0.49
3:L:66:GLY:HA3	3:L:71:PHE:HA	1.94	0.49
1:G:232:GLU:HB2	1:G:271:LYS:HE2	1.93	0.49
2:A:29:PHE:CE1	2:A:71:ARG:HD2	2.48	0.49
1:E:294:ILE:HD11	1:E:449:ILE:HD11	1.95	0.49
1:E:207:LYS:HE2	1:E:436:ALA:HB3	1.93	0.49
1:G:386:ASN:O	1:G:416:LEU:HD22	2.13	0.49
2:H:141:LEU:CD2	2:H:143:LYS:HB2	2.43	0.49
1:G:336:THR:O	1:G:340:ASN:ND2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:89:VAL:HG22	2:H:108:THR:HG22	1.95	0.49
3:L:46:LEU:HD21	3:L:49:HIS:CD2	2.48	0.49
4:E:501:NAG:C1	4:E:501:NAG:O7	2.62	0.48
3:D:147:GLN:HG2	3:D:154:LEU:HD21	1.94	0.48
3:L:108:ARG:HG2	3:L:109:THR:N	2.27	0.48
1:G:432:GLN:NE2	5:G:507:SO4:O2	2.44	0.48
3:L:65:ARG:HG2	3:L:66:GLY:H	1.79	0.48
2:A:50:LEU:C	2:A:50:LEU:HD12	2.34	0.48
1:E:297:THR:HG23	1:E:444:ARG:HG2	1.95	0.48
1:E:258:GLN:CG	1:E:470:PRO:HB2	2.44	0.48
2:A:66:ARG:NH2	2:A:86:ASP:OD2	2.45	0.48
1:E:65:LYS:HB3	1:E:115:SER:OG	2.14	0.48
3:D:35:TRP:HD1	3:D:48:ILE:HG21	1.78	0.48
3:L:49:HIS:CD2	3:L:55:ALA:HB2	2.49	0.48
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.49	0.47
1:G:343:HIS:O	1:G:346:VAL:HG12	2.13	0.47
1:E:69:TRP:CG	1:E:111:LEU:HG	2.49	0.47
2:H:100(E):LEU:HD13	3:L:49:HIS:ND1	2.29	0.47
3:D:50:GLY:O	3:D:51:PRO:C	2.52	0.47
2:A:47:TRP:CH2	2:A:49:GLY:HA2	2.50	0.47
2:A:96:GLY:HA2	2:A:100:VAL:CG2	2.45	0.46
3:D:21:LEU:C	3:D:21:LEU:HD12	2.36	0.46
1:G:453:ILE:HD12	1:G:472:GLY:HA2	1.96	0.46
1:G:427:TRP:HA	2:H:73:ARG:HH22	1.78	0.46
3:D:2:ILE:HG22	3:D:3:VAL:N	2.30	0.46
3:L:2:ILE:HG22	3:L:3:VAL:N	2.31	0.46
2:A:51:ILE:HD11	2:A:69:LEU:HB3	1.98	0.46
1:G:390:LEU:HD21	1:G:416:LEU:HD11	1.98	0.46
2:A:31:GLU:O	2:A:100:VAL:HG22	2.15	0.46
3:D:23:CYS:HB2	3:D:35:TRP:CH2	2.51	0.46
1:E:350:ARG:HD3	1:E:356:LYS:HB3	1.96	0.46
3:L:52:THR:CB	3:L:53:ASP:HA	2.46	0.46
1:E:342:LEU:O	1:E:346:VAL:HG13	2.16	0.46
3:D:55:ALA:HB1	3:D:56:PRO:HD2	1.98	0.45
1:E:279:ASN:HB3	1:E:282:LYS:HD2	1.98	0.45
3:L:105:GLU:OE1	3:L:173:TYR:OH	2.24	0.45
3:L:55:ALA:HB1	3:L:56:PRO:HD2	1.98	0.45
2:H:201:LYS:HB2	2:H:202:PRO:HD3	1.97	0.45
1:E:491:ILE:HG23	1:E:491:ILE:O	2.16	0.45
3:L:4:LEU:N	3:L:4:LEU:HD12	2.31	0.45
1:G:120:VAL:HG11	1:G:434:MET:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:THR:HG23	2:H:110:ILE:HA	1.98	0.45
2:A:50:LEU:HD12	2:A:50:LEU:O	2.17	0.45
1:E:326:ILE:HG21	1:E:440:ARG:CZ	2.47	0.45
1:E:258:GLN:HG2	1:E:470:PRO:HB2	1.99	0.45
3:L:21:LEU:HD12	3:L:21:LEU:N	2.32	0.45
2:H:51:ILE:HD12	2:H:78:VAL:HB	1.99	0.44
1:E:333:VAL:CG2	1:E:334:ASN:N	2.80	0.44
2:A:201:LYS:N	2:A:202:PRO:CD	2.80	0.44
1:E:120:VAL:HG22	1:E:121:LYS:N	2.33	0.44
3:L:21:LEU:HD23	3:L:102:THR:OG1	2.16	0.44
2:A:37:ILE:HA	2:A:48:LEU:HD12	1.99	0.44
1:G:390:LEU:HD11	1:G:416:LEU:HD11	1.99	0.44
1:G:120:VAL:HG21	1:G:434:MET:SD	2.58	0.43
1:G:258:GLN:HG2	1:G:470:PRO:HB2	2.00	0.43
1:E:386:ASN:HB3	1:E:417:PRO:HG2	2.01	0.43
1:E:286:VAL:HB	1:E:452:LEU:HB2	2.00	0.43
1:G:105:HIS:CE1	1:G:427:TRP:HZ3	2.37	0.43
3:D:21:LEU:CD1	3:D:35:TRP:CZ3	3.02	0.43
3:L:33:VAL:HG11	3:L:88:CYS:HB2	2.00	0.43
2:A:148:GLU:HB3	2:A:149:PRO:HA	2.01	0.43
2:H:201:LYS:N	2:H:202:PRO:CD	2.81	0.43
3:L:186:TYR:O	3:L:192:TYR:OH	2.30	0.43
3:L:48:ILE:HG12	3:L:64:ALA:CB	2.49	0.43
1:E:93:PHE:HB2	1:E:233:PHE:CZ	2.54	0.43
1:E:333:VAL:HG22	1:E:334:ASN:N	2.33	0.43
2:A:100:VAL:O	2:A:100(A):ALA:HB3	2.19	0.42
2:H:100(F):TYR:N	3:L:50:GLY:O	2.28	0.42
3:D:34:VAL:HG12	3:D:36:TYR:CE1	2.54	0.42
1:E:386:ASN:HD22	4:E:502:NAG:C7	2.32	0.42
1:G:258:GLN:CG	1:G:470:PRO:HB2	2.49	0.42
2:A:100(E):LEU:HD22	3:D:49:HIS:HB3	2.00	0.42
2:A:4:LEU:HD11	2:A:28:THR:HG21	2.01	0.42
3:D:197:THR:HG22	3:D:204:PRO:HG3	2.02	0.42
3:D:145:LYS:HB3	3:D:197:THR:OG1	2.20	0.42
1:G:295:ASN:CG	4:G:502:NAG:H2	2.40	0.42
2:H:66:ARG:HH22	2:H:86:ASP:CG	2.22	0.42
1:E:120:VAL:HG12	1:E:434:MET:HB2	2.01	0.42
1:E:48:ALA:CB	1:E:490:LYS:HB2	2.50	0.42
1:E:292:VAL:HB	1:E:449:ILE:HB	2.00	0.41
2:H:178:LEU:HD12	2:H:178:LEU:C	2.41	0.41
3:L:186:TYR:HA	3:L:192:TYR:OH	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:ASN:ND2	4:E:504:NAG:C1	2.84	0.41
2:A:22:CYS:HB3	2:A:78:VAL:HG23	2.02	0.41
1:G:461:THR:O	1:G:462:ASN:HB2	2.20	0.41
1:G:116:LEU:HD13	1:G:210:PHE:HE2	1.86	0.41
2:A:89:VAL:HG22	2:A:108:THR:HG22	2.02	0.41
2:H:119:PRO:HB3	2:H:145:TYR:HB3	2.03	0.41
2:H:29:PHE:CZ	2:H:71:ARG:HD2	2.55	0.41
3:L:4:LEU:HD11	3:L:90:GLU:CB	2.51	0.41
1:E:270:VAL:HG23	1:E:348:GLN:HG3	2.02	0.41
3:L:52:THR:HB	3:L:53:ASP:HA	2.02	0.41
1:E:120:VAL:CG1	1:E:434:MET:HB2	2.51	0.41
1:G:368:ASP:OD2	2:H:73:ARG:HD2	2.21	0.41
1:G:389:ASN:HB2	1:G:416:LEU:HD23	2.02	0.41
2:H:151:THR:HG23	2:H:199:ASN:HB3	2.03	0.41
1:G:69:TRP:CG	1:G:111:LEU:HG	2.56	0.40
2:A:55:GLY:O	2:A:57:LEU:CD1	2.69	0.40
1:G:116:LEU:HD22	1:G:210:PHE:CE2	2.56	0.40
1:E:109:ILE:HG12	1:E:428:GLN:HB2	2.02	0.40
1:G:93:PHE:CE2	1:G:487:LYS:HG2	2.57	0.40
2:H:151:THR:CG2	2:H:199:ASN:HB3	2.51	0.40
1:G:96:TRP:HE1	1:G:236:ILE:HD11	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	E	310/354 (88%)	295 (95%)	11 (4%)	4 (1%)	14	54
1	G	317/354 (90%)	299 (94%)	13 (4%)	5 (2%)	11	50
2	A	218/229 (95%)	209 (96%)	8 (4%)	1 (0%)	32	73
2	H	213/229 (93%)	206 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	211/213 (99%)	204 (97%)	4 (2%)	3 (1%)	13	52
3	L	210/213 (99%)	205 (98%)	5 (2%)	0	100	100
All	All	1479/1592 (93%)	1418 (96%)	48 (3%)	13 (1%)	20	63

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	465	ARG
3	D	2	ILE
3	D	53	ASP
1	G	118	PRO
1	G	120	VAL
1	G	357	LYS
1	E	45	TRP
1	E	464	THR
3	D	50	GLY
2	A	216	CYS
1	G	117	LYS
1	G	462	ASN
1	E	356	LYS

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	E	289/312 (93%)	284 (98%)	5 (2%)	66	87
1	G	292/312 (94%)	276 (94%)	16 (6%)	25	62
2	A	186/191 (97%)	182 (98%)	4 (2%)	57	83
2	H	181/191 (95%)	181 (100%)	0	100	100
3	D	185/185 (100%)	181 (98%)	4 (2%)	57	83
3	L	184/185 (100%)	181 (98%)	3 (2%)	68	87
All	All	1317/1376 (96%)	1285 (98%)	32 (2%)	54	82

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	89	VAL
1	G	92	GLU
1	G	114	GLN
1	G	116	LEU
1	G	117	LYS
1	G	119	CYS
1	G	123	THR
1	G	209	THR
1	G	255	VAL
1	G	268	LYS
1	G	278	THR
1	G	368	ASP
1	G	428	GLN
1	G	453	ILE
1	G	463	SER
1	G	490	LYS
3	L	20	THR
3	L	52	THR
3	L	90	GLU
1	E	119	CYS
1	E	209	THR
1	E	332	ASN
1	E	365	THR
1	E	467	THR
2	A	57	LEU
2	A	111	VAL
2	A	184	VAL
2	A	218	LYS
3	D	1	GLU
3	D	20	THR
3	D	52	THR
3	D	90	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	241	ASN
3	D	49	HIS

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 ⓘ

28 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	$\# Z > 2$
5	SO4	A	301	-	4,4,4	0.17	0	6,6,6	0.18	0
5	SO4	D	301	-	4,4,4	0.14	0	6,6,6	0.16	0
5	SO4	D	302	-	4,4,4	0.11	0	6,6,6	0.12	0
5	SO4	D	303	-	4,4,4	0.17	0	6,6,6	0.10	0
5	SO4	D	304	-	4,4,4	0.15	0	6,6,6	0.23	0
4	NAG	E	501	1	14,14,15	0.52	0	15,19,21	0.99	1 (6%)
4	NAG	E	502	1	14,14,15	0.33	0	15,19,21	0.56	0
4	NAG	E	503	1	14,14,15	0.43	0	15,19,21	0.48	0
4	NAG	E	504	-	14,14,15	0.22	0	15,19,21	0.64	1 (6%)
4	NAG	E	505	-	14,14,15	0.30	0	15,19,21	0.70	1 (6%)
5	SO4	E	506	-	4,4,4	0.14	0	6,6,6	0.14	0
6	EDO	E	507	-	3,3,3	0.49	0	2,2,2	0.30	0
4	NAG	G	501	1	14,14,15	0.83	1 (7%)	15,19,21	1.03	1 (6%)
4	NAG	G	502	-	14,14,15	0.43	0	15,19,21	0.67	0
4	NAG	G	503	1	14,14,15	0.31	0	15,19,21	0.77	1 (6%)
4	NAG	G	504	1	14,14,15	0.64	1 (7%)	15,19,21	0.85	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	505	1	14,14,15	0.41	0	15,19,21	0.51	0
4	NAG	G	506	1	14,14,15	0.41	0	15,19,21	0.55	0
5	SO4	G	507	-	4,4,4	0.18	0	6,6,6	0.08	0
6	EDO	G	508	-	3,3,3	0.63	0	2,2,2	0.07	0
6	EDO	G	509	-	3,3,3	0.57	0	2,2,2	0.18	0
6	EDO	G	510	-	3,3,3	0.54	0	2,2,2	0.16	0
5	SO4	G	511	-	4,4,4	0.18	0	6,6,6	0.17	0
5	SO4	G	512	-	4,4,4	0.17	0	6,6,6	0.29	0
6	EDO	G	513	-	3,3,3	0.28	0	2,2,2	0.62	0
5	SO4	L	401	-	4,4,4	0.14	0	6,6,6	0.15	0
5	SO4	L	402	-	4,4,4	0.16	0	6,6,6	0.16	0
5	SO4	L	403	-	4,4,4	0.18	0	6,6,6	0.30	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
5	SO4	A	301	-	-	0/0/0/0	0/0/0/0
5	SO4	D	301	-	-	0/0/0/0	0/0/0/0
5	SO4	D	302	-	-	0/0/0/0	0/0/0/0
5	SO4	D	303	-	-	0/0/0/0	0/0/0/0
5	SO4	D	304	-	-	0/0/0/0	0/0/0/0
4	NAG	E	501	1	-	0/6/23/26	0/1/1/1
4	NAG	E	502	1	-	0/6/23/26	0/1/1/1
4	NAG	E	503	1	-	0/6/23/26	0/1/1/1
4	NAG	E	504	-	-	0/6/23/26	0/1/1/1
4	NAG	E	505	-	-	0/6/23/26	0/1/1/1
5	SO4	E	506	-	-	0/0/0/0	0/0/0/0
6	EDO	E	507	-	-	0/1/1/1	0/0/0/0
4	NAG	G	501	1	-	0/6/23/26	0/1/1/1
4	NAG	G	502	-	-	0/6/23/26	0/1/1/1
4	NAG	G	503	1	-	0/6/23/26	0/1/1/1
4	NAG	G	504	1	-	0/6/23/26	0/1/1/1
4	NAG	G	505	1	-	0/6/23/26	0/1/1/1
4	NAG	G	506	1	-	0/6/23/26	0/1/1/1
5	SO4	G	507	-	-	0/0/0/0	0/0/0/0
6	EDO	G	508	-	-	0/1/1/1	0/0/0/0
6	EDO	G	509	-	-	0/1/1/1	0/0/0/0
6	EDO	G	510	-	-	0/1/1/1	0/0/0/0
5	SO4	G	511	-	-	0/0/0/0	0/0/0/0
5	SO4	G	512	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	G	513	-	-	0/1/1/1	0/0/0/0
5	SO4	L	401	-	-	0/0/0/0	0/0/0/0
5	SO4	L	402	-	-	0/0/0/0	0/0/0/0
5	SO4	L	403	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	504	NAG	O5-C1	-2.19	1.40	1.43
4	G	501	NAG	C1-C2	2.33	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	504	NAG	C1-O5-C5	2.06	115.00	112.17
4	G	504	NAG	C1-O5-C5	2.13	115.11	112.17
4	E	505	NAG	C1-O5-C5	2.29	115.32	112.17
4	G	503	NAG	C1-O5-C5	2.52	115.64	112.17
4	E	501	NAG	C2-N2-C7	2.83	127.07	122.94
4	G	501	NAG	C1-O5-C5	3.59	117.11	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	301	SO4	1	0
4	E	501	NAG	2	0
4	E	502	NAG	1	0
4	E	503	NAG	1	0
4	E	504	NAG	2	0
4	G	502	NAG	1	0
4	G	504	NAG	1	0
4	G	505	NAG	1	0
4	G	506	NAG	1	0
5	G	507	SO4	1	0
6	G	513	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	E	320/354 (90%)	0.60	29 (9%)	10 11	83, 141, 212, 286	0
1	G	325/354 (91%)	0.45	24 (7%)	15 15	70, 120, 193, 298	0
2	A	222/229 (96%)	0.12	2 (0%)	84 78	70, 100, 158, 284	0
2	H	217/229 (94%)	0.20	12 (5%)	26 23	59, 102, 176, 272	0
3	D	213/213 (100%)	0.27	8 (3%)	41 37	82, 122, 156, 181	0
3	L	212/213 (99%)	0.41	8 (3%)	41 37	65, 116, 164, 199	0
All	All	1509/1592 (94%)	0.37	83 (5%)	26 23	59, 118, 187, 298	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	128	SER	7.8
1	E	45	TRP	6.9
1	E	123	THR	6.7
1	G	58	ALA	5.7
1	E	44	VAL	5.2
1	E	205	CYS	5.1
1	G	442	VAL	4.7
1	E	353	PHE	4.7
1	E	119	CYS	4.6
1	E	413	THR	4.5
1	E	366	GLY	4.4
1	G	45	TRP	4.1
3	L	214	CYS	4.0
2	H	159	LEU	3.9
1	G	59	LYS	3.7
1	E	477	ASP	3.7
1	E	359	ILE	3.6
1	E	352	HIS	3.5
1	G	61	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	464	THR	3.5
3	L	213	GLU	3.4
1	G	463	SER	3.4
1	E	478	ASN	3.3
1	G	328	GLN	3.3
2	H	191	THR	3.3
1	G	60	ALA	3.2
3	L	187	GLU	3.0
1	E	442	VAL	3.0
2	H	139	GLY	3.0
1	E	299	PRO	2.9
3	D	60	ASP	2.9
2	H	140	CYS	2.9
3	L	119	PRO	2.9
3	D	52	THR	2.8
3	D	110	VAL	2.8
1	E	300	ASN	2.8
1	E	62	GLU	2.8
1	G	57	ASP	2.8
1	G	357	LYS	2.8
1	E	47	GLU	2.7
2	H	158	ALA	2.7
3	D	29	GLY	2.6
1	G	67	ASN	2.6
3	L	15	PRO	2.6
1	E	295	ASN	2.6
3	L	212	GLY	2.6
1	E	463	SER	2.6
1	E	122	LEU	2.5
1	E	46	LYS	2.4
1	E	357	THR	2.4
2	H	156	SER	2.4
3	L	201	LEU	2.4
2	A	204	ASN	2.4
2	H	179	SER	2.3
2	H	187	SER	2.3
1	E	89	VAL	2.3
1	E	356	LYS	2.3
3	L	60	ASP	2.3
1	E	58	ALA	2.3
1	G	239	CYS	2.3
1	G	122	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	365	THR	2.2
1	G	440	ARG	2.2
1	G	267	GLU	2.2
1	E	117	LYS	2.2
3	D	27	GLN	2.2
1	G	90	THR	2.2
1	E	415	ILE	2.2
1	G	238	PRO	2.1
2	H	157	GLY	2.1
1	G	330	HIS	2.1
1	G	478	ASN	2.1
3	D	30	LEU	2.1
2	H	193	THR	2.1
1	E	256	SER	2.1
1	G	47	GLU	2.1
3	D	12	SER	2.1
3	D	154	LEU	2.1
1	G	119	CYS	2.0
1	G	444	ARG	2.0
2	H	116	THR	2.0
1	E	116	LEU	2.0
2	H	195	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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(\AA^2)	Q<0.9
6	EDO	G	509	4/4	0.60	0.80	7.76	94,113,121,122	0
4	NAG	E	503	14/15	0.79	0.41	7.44	133,166,199,199	0
5	SO4	L	403	5/5	0.55	0.56	7.09	254,255,256,257	0
5	SO4	A	301	5/5	0.58	0.56	6.65	199,200,200,201	0
6	EDO	G	513	4/4	0.71	0.78	6.29	151,182,183,183	0
5	SO4	D	304	5/5	0.50	0.60	6.26	263,264,264,265	0
6	EDO	E	507	4/4	0.82	0.37	3.30	94,113,118,118	0
4	NAG	E	502	14/15	0.83	0.41	3.00	119,150,200,200	0
5	SO4	G	512	5/5	0.71	0.63	2.64	267,268,269,271	0
4	NAG	G	504	14/15	0.95	0.33	2.62	107,156,203,203	0
5	SO4	D	302	5/5	0.73	0.39	2.46	184,185,186,186	0
4	NAG	G	505	14/15	0.76	0.41	1.43	171,190,227,227	0
5	SO4	D	301	5/5	0.84	0.35	1.38	171,172,173,174	0
4	NAG	E	501	14/15	0.74	0.44	1.22	150,180,194,194	0
4	NAG	E	505	14/15	0.72	0.36	1.21	139,192,248,248	0
4	NAG	G	503	14/15	0.94	0.29	0.92	130,137,163,164	0
5	SO4	G	507	5/5	0.84	0.36	0.76	193,193,195,195	0
5	SO4	E	506	5/5	0.77	0.35	0.72	176,176,177,179	0
5	SO4	L	401	5/5	0.77	0.29	0.65	183,183,185,186	0
4	NAG	G	506	14/15	0.52	0.31	-0.23	141,190,230,233	0
4	NAG	G	502	14/15	0.68	0.33	-0.53	121,161,198,200	0
4	NAG	E	504	14/15	0.77	0.27	-0.54	147,185,222,228	0
4	NAG	G	501	14/15	0.92	0.20	-0.58	73,155,186,189	0
5	SO4	G	511	5/5	0.82	0.23	-0.72	154,155,157,159	0
6	EDO	G	508	4/4	0.81	0.28	-0.76	90,108,114,114	0
5	SO4	L	402	5/5	0.81	0.18	-	189,190,190,192	0
5	SO4	D	303	5/5	0.71	0.36	-	187,188,189,189	0
6	EDO	G	510	4/4	0.59	0.42	-	95,114,123,123	0

6.5 Other polymers [i](#)

There are no such residues in this entry.