



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:09 PM GMT

PDB ID : 3T24
Title : Crystal structure of Pseudomonas aeruginosa OpdQ
Authors : van den Berg, B.; Eren, E.
Deposited on : 2011-07-22
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

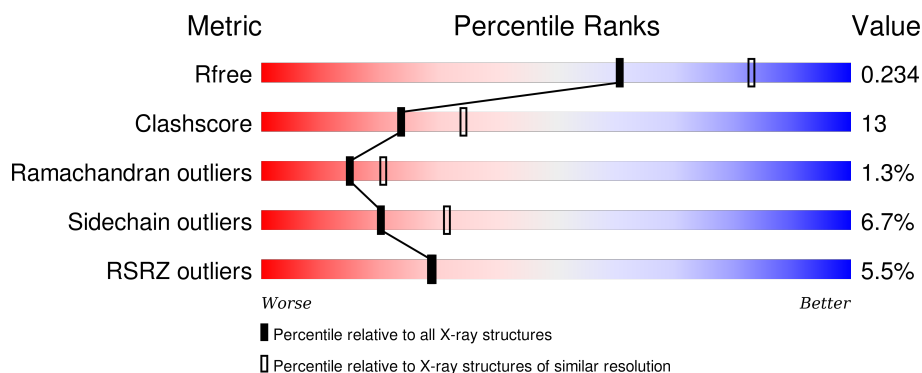
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	A	401	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 71%, yellow 19%, orange 6%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 71% 19% • 6% </div> </div>
1	B	401	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 5%, green 66%, yellow 23%, orange 8%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 66% 23% • 8% </div> </div>
1	C	401	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 9%, green 70%, yellow 18%, orange 8%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 9% 70% 18% • 8% </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
2	SO4	A	400	-	-	-	X
2	SO4	B	395	-	-	X	-
2	SO4	B	396	-	-	-	X
2	SO4	C	395	-	-	X	-
3	C8E	A	401	-	-	-	X
3	C8E	A	403	-	-	X	X
3	C8E	A	404	-	-	-	X
3	C8E	B	399	-	-	-	X
3	C8E	B	402	-	-	-	X
3	C8E	C	398	-	-	-	X
3	C8E	C	399	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9050 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 porin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2955	1869	501	577	8			
1	B	368	Total	C	N	O	S	0	0	0
			2846	1799	482	557	8			
1	C	367	Total	C	N	O	S	0	0	0
			2777	1745	474	550	8			

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



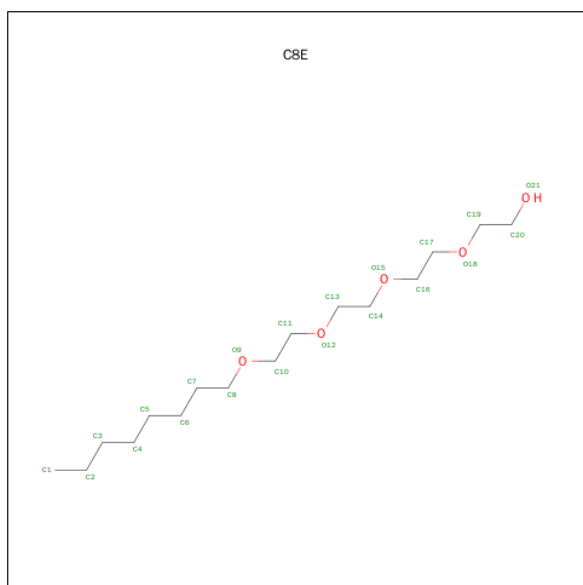
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	14	4		
3	A	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	11	5		
3	A	1	Total	C	O	0	0
			12	10	2		
3	A	1	Total	C	O	0	0
			15	10	5		
3	B	1	Total	C	O	0	0
			19	14	5		
3	B	1	Total	C	O	0	0
			20	15	5		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			11	10	1		
3	B	1	Total	C	O	0	0
			18	14	4		
3	C	1	Total	C	O	0	0
			14	10	4		
3	C	1	Total	C	O	0	0
			11	9	2		

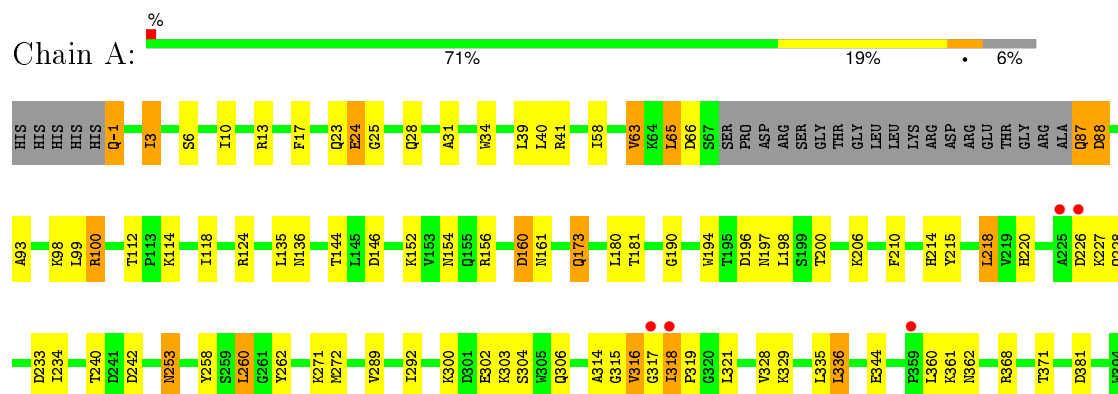
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	118	Total	O	0	0
			118	118		
4	B	82	Total	O	0	0
			82	82		
4	C	38	Total	O	0	0
			38	38		

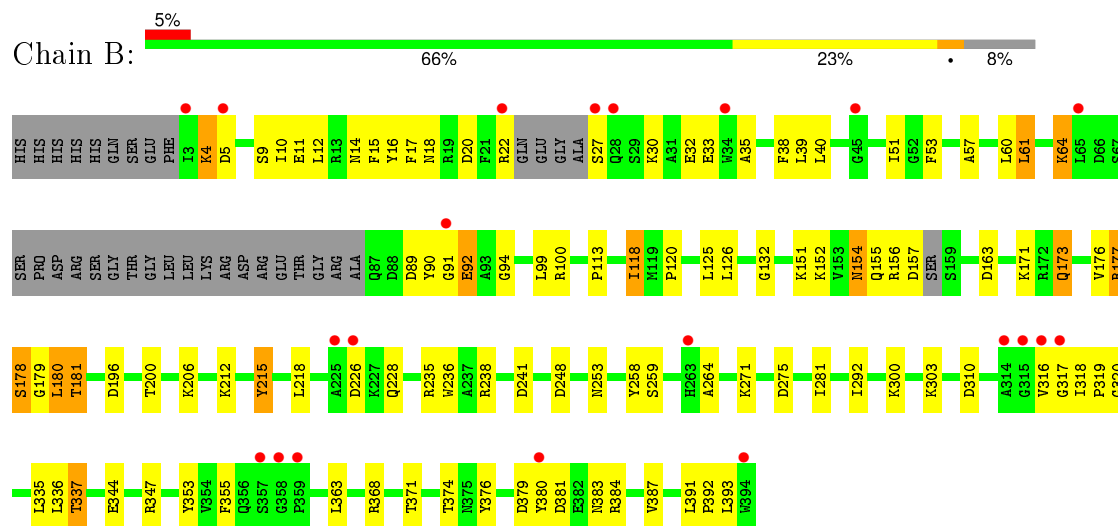
3 Residue-property plots

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.

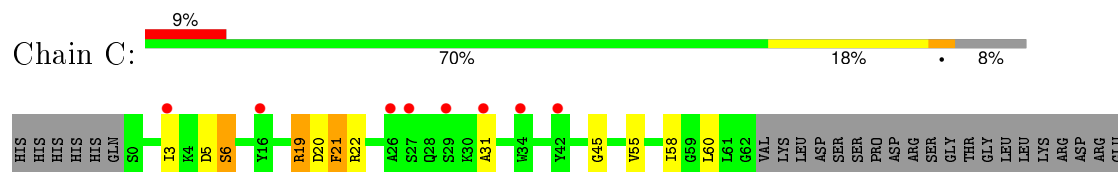
• Molecule 1: porin

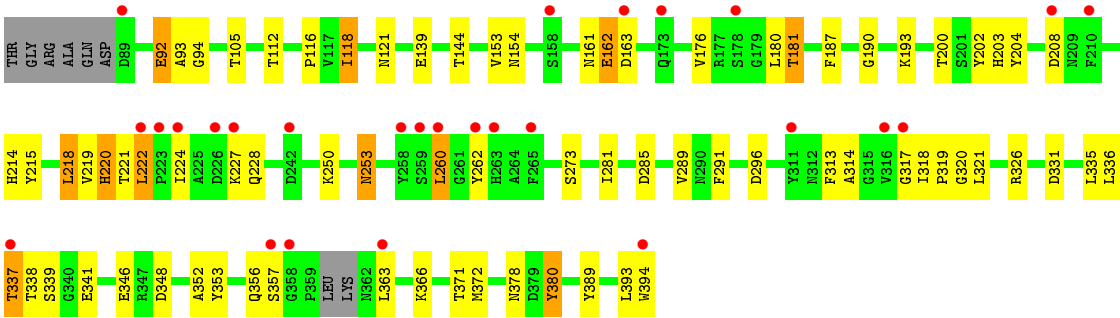


• Molecule 1: porin



• Molecule 1: porin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.72Å 78.46Å 97.52Å 77.76° 81.50° 70.04°	Depositor
Resolution (Å)	14.98 – 2.40 40.77 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.3 (14.98-2.40) 88.3 (40.77-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.203 , 0.242 0.192 , 0.234	Depositor DCC
R_{free} test set	1867 reflections (2.91%)	DCC
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 68172 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9050	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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, 0.375 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: C8E, 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	0.47	0/3019	0.60	0/4080
1	B	0.43	0/2906	0.58	1/3927 (0.0%)
1	C	0.35	0/2836	0.50	0/3837
All	All	0.42	0/8761	0.56	1/11844 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	LEU	CA-CB-CG	5.20	127.27	115.30

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	2955	0	2813	86	0
1	B	2846	0	2665	75	0
1	C	2777	0	2534	63	0
2	A	30	0	0	2	0
2	B	15	0	0	2	0
2	C	15	0	0	2	0
3	A	71	0	103	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	78	0	112	6	0
3	C	25	0	30	4	0
4	A	118	0	0	6	0
4	B	82	0	0	3	0
4	C	38	0	0	2	0
All	All	9050	0	8257	226	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 13.

All (226) 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:C:22:ARG:NH1	2:C:395:SO4:O1	1.94	1.00
1:A:100:ARG:HH11	1:A:100:ARG:HG2	1.34	0.92
1:A:-1:GLN:O	1:A:3:ILE:HG22	1.76	0.84
1:A:24:GLU:HG2	1:A:25:GLY:H	1.44	0.83
1:B:228:GLN:OE1	1:B:258:TYR:OH	1.96	0.82
1:B:374:THR:OG1	4:B:436:HOH:O	1.99	0.79
1:B:163:ASP:HB3	1:B:181:THR:HG23	1.64	0.79
1:A:173:GLN:HB2	1:A:336:LEU:HD21	1.65	0.78
1:A:368:ARG:NH1	4:A:482:HOH:O	2.16	0.77
1:C:220:HIS:CE1	1:C:222:LEU:HD22	2.20	0.76
1:A:100:ARG:NH1	4:A:443:HOH:O	2.20	0.74
1:C:363:LEU:HD12	1:C:389:TYR:HB2	1.67	0.73
1:A:24:GLU:CG	1:A:25:GLY:H	2.01	0.73
2:A:399:SO4:O3	4:A:520:HOH:O	2.08	0.72
1:A:220:HIS:HE1	3:A:403:C8E:H191	1.55	0.71
1:A:100:ARG:CG	1:A:100:ARG:HH11	2.02	0.70
1:A:316:VAL:HG23	1:A:317:GLY:N	2.05	0.70
1:A:306:GLN:HB2	1:A:328:VAL:HG22	1.73	0.70
1:A:87:GLN:O	1:A:88:ASP:HB2	1.91	0.70
1:A:41:ARG:HG2	1:A:58:ILE:CD1	2.22	0.69
1:C:92:GLU:HG3	1:C:93:ALA:H	1.58	0.69
1:A:253:ASN:HB2	1:A:289:VAL:HG22	1.74	0.69
2:A:398:SO4:O1	4:A:454:HOH:O	2.08	0.68
1:A:112:THR:O	1:A:112:THR:HG23	1.92	0.68
1:B:376:TYR:N	4:B:436:HOH:O	2.26	0.68
1:B:200:THR:HB	3:B:398:C8E:H61	1.76	0.68
1:A:173:GLN:HG2	1:A:300:LYS:HD2	1.77	0.67
1:A:98:LYS:C	1:A:99:LEU:HD12	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:HA	1:A:88:ASP:O	1.96	0.66
1:A:160:ASP:N	1:A:160:ASP:OD1	2.27	0.66
1:B:200:THR:OG1	3:B:398:C8E:H81	1.97	0.65
1:C:363:LEU:CD1	1:C:389:TYR:HB2	2.27	0.64
1:A:100:ARG:NH1	1:A:100:ARG:HG2	2.07	0.64
1:A:10:ILE:HD13	1:A:40:LEU:HG	1.78	0.64
1:C:92:GLU:HG3	1:C:93:ALA:N	2.13	0.63
1:B:371:THR:HG23	1:B:381:ASP:OD2	1.99	0.63
1:B:53:PHE:CE1	1:B:99:LEU:HD13	2.35	0.62
3:A:404:C8E:H42	3:A:404:C8E:H81	1.82	0.62
1:B:173:GLN:HG3	1:B:173:GLN:O	1.99	0.62
1:B:20:ASP:O	1:B:380:TYR:HB2	2.00	0.61
1:C:116:PRO:HG2	1:C:203:HIS:CD2	2.35	0.61
1:A:13:ARG:NH1	1:A:124:ARG:O	2.32	0.61
1:A:23:GLN:O	1:A:24:GLU:HB3	2.00	0.60
1:B:335:LEU:O	1:B:337:THR:N	2.33	0.60
1:B:90:TYR:CE1	1:B:126:LEU:HD12	2.36	0.60
1:A:318:ILE:HG22	1:A:321:LEU:HB3	1.82	0.60
1:B:17:PHE:HD1	1:B:384:ARG:HG2	1.66	0.60
1:C:22:ARG:NH1	2:C:395:SO4:S	2.75	0.60
1:B:215:TYR:HE2	1:B:235:ARG:HB3	1.68	0.59
1:A:173:GLN:HG3	1:A:173:GLN:O	2.03	0.59
1:C:319:PRO:HB2	1:C:356:GLN:OE1	2.03	0.59
1:A:316:VAL:HG23	1:A:317:GLY:H	1.67	0.58
1:B:156:ARG:O	4:B:485:HOH:O	2.17	0.58
1:B:35:ALA:HB1	1:B:125:LEU:HD22	1.85	0.58
1:C:227:LYS:O	1:C:260:LEU:HA	2.03	0.58
1:A:318:ILE:HG22	1:A:321:LEU:CB	2.34	0.58
1:B:51:ILE:CG2	1:B:99:LEU:HD11	2.34	0.58
1:B:379:ASP:O	1:B:380:TYR:HB3	2.03	0.58
1:A:198:LEU:HD23	3:A:403:C8E:H132	1.85	0.57
1:C:260:LEU:HD13	1:C:260:LEU:O	2.04	0.57
1:C:224:ILE:HD11	1:C:228:GLN:HG2	1.85	0.57
1:B:10:ILE:HG12	1:B:393:LEU:HD21	1.85	0.57
1:C:163:ASP:HB3	1:C:181:THR:HG23	1.85	0.57
1:A:197:ASN:HB2	3:A:403:C8E:H202	1.87	0.57
1:C:336:LEU:O	1:C:337:THR:CB	2.53	0.57
1:A:23:GLN:OE1	1:A:28:GLN:HG2	2.05	0.57
1:A:24:GLU:CG	1:A:25:GLY:N	2.67	0.57
1:B:173:GLN:HG2	1:B:300:LYS:HD2	1.86	0.57
1:B:218:LEU:HD23	1:B:218:LEU:C	2.26	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLU:HG2	1:A:25:GLY:N	2.17	0.56
1:A:41:ARG:HG2	1:A:58:ILE:HD11	1.87	0.56
1:C:317:GLY:C	1:C:319:PRO:HD3	2.26	0.56
1:C:154:ASN:HB2	1:C:161:ASN:OD1	2.06	0.55
1:B:178:SER:OG	2:B:395:SO4:O3	2.24	0.55
1:C:19:ARG:HB2	1:C:31:ALA:HB3	1.89	0.55
1:A:271:LYS:HD3	1:A:303:LYS:CG	2.36	0.55
1:C:112:THR:O	1:C:112:THR:HG23	2.07	0.54
1:C:393:LEU:O	1:C:394:TRP:HB3	2.07	0.54
1:C:202:TYR:OH	1:C:214:HIS:ND1	2.40	0.54
1:A:258:TYR:HE2	1:A:260:LEU:HD23	1.72	0.54
1:B:344:GLU:HB3	1:B:374:THR:HG22	1.89	0.54
1:A:41:ARG:HG2	1:A:58:ILE:HD12	1.88	0.54
1:C:331:ASP:HB2	1:C:341:GLU:OE1	2.08	0.54
1:A:335:LEU:O	1:A:336:LEU:HB2	2.08	0.53
1:A:99:LEU:HD12	1:A:99:LEU:N	2.24	0.53
1:A:24:GLU:OE2	1:A:25:GLY:N	2.42	0.53
1:A:262:TYR:CE2	1:A:315:GLY:HA2	2.44	0.52
1:B:163:ASP:CB	1:B:181:THR:HG23	2.38	0.52
1:A:31:ALA:HB2	1:B:179:GLY:HA3	1.90	0.52
1:B:57:ALA:HA	1:B:94:GLY:O	2.09	0.52
1:B:271:LYS:HE2	1:B:303:LYS:HE2	1.90	0.52
1:B:18:ASN:OD1	1:B:383:ASN:HB2	2.09	0.52
1:B:132:GLY:HA2	3:B:401:C8E:H102	1.92	0.52
1:C:253:ASN:HB2	1:C:289:VAL:HG22	1.92	0.52
1:A:124:ARG:HG2	1:A:156:ARG:NH1	2.24	0.52
1:C:262:TYR:CE1	1:C:314:ALA:HB3	2.45	0.52
1:B:27:SER:OG	1:B:30:LYS:HE3	2.10	0.52
1:B:61:LEU:HD11	3:B:400:C8E:H171	1.91	0.52
1:A:124:ARG:HG3	1:A:156:ARG:HD2	1.92	0.51
1:A:173:GLN:CB	1:A:336:LEU:HD21	2.39	0.51
1:A:124:ARG:CG	1:A:156:ARG:HD2	2.41	0.51
1:A:39:LEU:HD12	1:A:39:LEU:N	2.26	0.51
1:A:214:HIS:HD2	4:A:516:HOH:O	1.93	0.51
1:C:21:PHE:CD1	1:C:378:ASN:HB3	2.46	0.51
1:B:173:GLN:CG	1:B:173:GLN:O	2.59	0.51
1:B:91:GLY:O	1:B:92:GLU:HB2	2.10	0.51
1:C:326:ARG:HG2	1:C:348:ASP:HB2	1.93	0.51
1:A:228:GLN:OE1	1:A:258:TYR:OH	2.26	0.51
1:B:200:THR:CB	3:B:398:C8E:H61	2.41	0.50
1:C:60:LEU:N	1:C:92:GLU:O	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:VAL:HG23	1:B:318:ILE:HD12	1.93	0.50
1:A:318:ILE:H	1:A:319:PRO:HD3	1.75	0.50
1:C:250:LYS:HB2	1:C:273:SER:HB2	1.93	0.50
1:B:10:ILE:HB	1:B:391:LEU:HD21	1.94	0.50
1:C:21:PHE:CE1	1:C:378:ASN:HB3	2.47	0.49
1:C:228:GLN:HG3	1:C:260:LEU:HB3	1.93	0.49
1:B:39:LEU:HG	1:B:60:LEU:HD22	1.94	0.49
1:C:200:THR:CB	3:C:399:C8E:H132	2.43	0.49
1:A:258:TYR:CE2	1:A:260:LEU:HD23	2.47	0.49
1:C:139:GLU:HB3	3:C:398:C8E:H132	1.94	0.48
1:B:16:TYR:OH	1:B:32:GLU:OE2	2.31	0.48
1:C:338:THR:HG22	1:C:339:SER:N	2.28	0.48
1:B:10:ILE:HD11	1:B:40:LEU:HD13	1.96	0.48
1:B:320:GLY:O	1:B:353:TYR:HA	2.14	0.48
1:C:20:ASP:O	1:C:380:TYR:HA	2.13	0.47
1:C:200:THR:HB	3:C:399:C8E:H132	1.96	0.47
1:A:194:TRP:CZ2	3:A:403:C8E:H81	2.49	0.47
1:A:262:TYR:CD2	1:A:315:GLY:HA2	2.49	0.47
1:A:173:GLN:CG	1:A:173:GLN:O	2.63	0.47
1:A:112:THR:CG2	1:A:112:THR:O	2.63	0.47
1:A:220:HIS:CE1	3:A:403:C8E:H191	2.44	0.47
1:B:61:LEU:CD1	3:B:400:C8E:H171	2.45	0.47
1:A:314:ALA:C	1:A:316:VAL:N	2.68	0.46
1:C:200:THR:OG1	3:C:399:C8E:H132	2.16	0.46
1:B:33:GLU:OE2	1:B:64:LYS:HD3	2.14	0.46
1:C:262:TYR:HE1	1:C:314:ALA:HB3	1.80	0.46
1:A:135:LEU:O	1:A:146:ASP:HA	2.15	0.46
1:B:22:ARG:HD2	1:B:381:ASP:OD1	2.16	0.46
1:B:264:ALA:HB3	1:B:310:ASP:HB2	1.97	0.46
1:C:356:GLN:O	1:C:357:SER:HB3	2.16	0.46
1:B:14:ASN:HB2	1:B:387:VAL:HB	1.97	0.46
1:B:60:LEU:HB3	1:B:126:LEU:HD22	1.97	0.45
1:B:39:LEU:N	1:B:39:LEU:HD12	2.31	0.45
1:C:181:THR:O	4:C:430:HOH:O	2.21	0.45
1:B:9:SER:O	1:B:10:ILE:HD13	2.17	0.45
1:C:346:GLU:HA	1:C:371:THR:O	2.16	0.45
1:A:234:ILE:N	1:A:234:ILE:HD12	2.31	0.45
1:B:53:PHE:CD1	1:B:99:LEU:HD13	2.52	0.45
1:B:317:GLY:C	1:B:319:PRO:HD3	2.37	0.45
1:A:314:ALA:C	1:A:316:VAL:H	2.19	0.45
1:A:87:GLN:O	1:A:88:ASP:CB	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:VAL:CG1	1:C:180:LEU:HB3	2.47	0.45
1:B:368:ARG:HB2	1:B:384:ARG:HB2	1.99	0.45
1:C:218:LEU:C	1:C:218:LEU:HD12	2.37	0.45
1:B:236:TRP:CH2	1:B:238:ARG:HB2	2.51	0.45
1:C:313:PHE:HD2	1:C:321:LEU:O	1.99	0.45
1:A:371:THR:HG23	1:A:381:ASP:OD2	2.17	0.45
1:B:15:PHE:CZ	1:B:17:PHE:HB2	2.52	0.44
1:A:31:ALA:HB2	1:B:179:GLY:CA	2.48	0.44
1:A:206:LYS:HE3	1:A:242:ASP:OD2	2.17	0.44
1:A:58:ILE:O	1:A:93:ALA:HA	2.18	0.44
1:C:218:LEU:HD12	1:C:219:VAL:N	2.33	0.44
1:A:304:SER:HA	1:A:329:LYS:O	2.18	0.44
1:A:154:ASN:HB2	1:A:161:ASN:OD1	2.18	0.44
1:C:58:ILE:O	1:C:94:GLY:N	2.47	0.44
1:A:200:THR:HG22	1:A:218:LEU:HD22	1.99	0.44
1:B:113:PRO:O	1:B:120:PRO:CD	2.65	0.44
1:B:177:ARG:NH1	2:B:395:SO4:O1	2.51	0.44
1:C:187:PHE:HA	1:C:204:TYR:O	2.17	0.44
1:B:206:LYS:CD	1:B:212:LYS:HG2	2.47	0.44
1:A:23:GLN:HB3	1:A:28:GLN:OE1	2.18	0.43
1:B:228:GLN:HA	1:B:259:SER:O	2.18	0.43
1:A:34:TRP:CE2	1:A:65:LEU:HD23	2.53	0.43
1:C:352:ALA:HB2	1:C:366:LYS:HE3	2.00	0.43
1:A:124:ARG:HB3	4:A:511:HOH:O	2.17	0.43
1:C:319:PRO:HB2	1:C:356:GLN:CD	2.39	0.43
1:C:144:THR:O	1:C:190:GLY:HA2	2.18	0.43
1:A:198:LEU:CD2	3:A:403:C8E:H132	2.47	0.43
1:A:262:TYR:CD2	1:A:315:GLY:CA	3.02	0.43
1:C:321:LEU:HB2	1:C:353:TYR:CD1	2.54	0.43
1:C:320:GLY:O	1:C:353:TYR:HA	2.19	0.43
1:A:226:ASP:HA	1:A:227:LYS:HA	1.43	0.43
1:B:155:GLN:HA	1:B:155:GLN:OE1	2.18	0.43
1:C:220:HIS:HD2	4:C:412:HOH:O	2.01	0.43
1:C:3:ILE:O	1:C:6:SER:HB2	2.19	0.43
1:C:193:LYS:HE2	1:C:193:LYS:HB3	1.67	0.43
1:A:197:ASN:CB	3:A:403:C8E:H202	2.48	0.42
1:A:233:ASP:C	1:A:234:ILE:HD12	2.40	0.42
1:B:4:LYS:HA	1:B:5:ASP:C	2.40	0.42
1:C:121:ASN:ND2	1:C:285:ASP:OD1	2.52	0.42
1:C:378:ASN:HB2	1:C:380:TYR:CZ	2.54	0.42
1:A:65:LEU:O	1:A:66:ASP:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:N	1:A:319:PRO:HD3	2.33	0.42
1:C:118:ILE:HD13	1:C:281:ILE:HD12	2.01	0.42
1:B:391:LEU:HA	1:B:392:PRO:HD3	1.90	0.42
1:B:355:PHE:CD2	1:B:363:LEU:HD23	2.55	0.42
1:B:163:ASP:CB	1:B:181:THR:CG2	2.98	0.42
3:A:403:C8E:H171	3:A:403:C8E:H142	1.53	0.42
1:A:361:LYS:O	1:A:362:ASN:HB2	2.20	0.42
1:B:11:GLU:HB3	1:B:39:LEU:HB2	2.01	0.41
1:B:17:PHE:CD1	1:B:384:ARG:HG2	2.52	0.41
1:B:176:VAL:HG12	1:B:177:ARG:N	2.34	0.41
1:B:10:ILE:HB	1:B:391:LEU:CD2	2.50	0.41
1:C:346:GLU:HG3	1:C:371:THR:O	2.20	0.41
1:A:144:THR:O	1:A:190:GLY:HA2	2.21	0.41
1:B:173:GLN:HG2	1:B:275:ASP:O	2.20	0.41
1:A:318:ILE:HG22	1:A:318:ILE:O	2.20	0.41
1:B:173:GLN:CG	1:B:275:ASP:O	2.69	0.41
1:C:21:PHE:C	1:C:21:PHE:CD1	2.93	0.41
1:A:152:LYS:HB3	1:A:161:ASN:HB3	2.02	0.41
1:C:5:ASP:HB2	1:C:45:GLY:HA3	2.02	0.41
1:C:153:VAL:O	1:C:162:GLU:HG3	2.21	0.41
1:B:118:ILE:HD13	1:B:281:ILE:HD12	2.02	0.41
1:A:220:HIS:HE1	3:A:403:C8E:C19	2.27	0.41
1:B:38:PHE:C	1:B:39:LEU:HD12	2.41	0.41
1:B:154:ASN:O	1:B:154:ASN:OD1	2.39	0.41
1:A:271:LYS:HD2	1:A:272:MET:O	2.20	0.41
1:A:180:LEU:HD23	1:A:210:PHE:CZ	2.56	0.41
1:B:171:LYS:HA	1:B:171:LYS:HD3	1.88	0.40
1:C:92:GLU:CG	1:C:93:ALA:N	2.82	0.40
1:C:318:ILE:N	1:C:319:PRO:HD3	2.36	0.40
1:C:291:PHE:HA	1:C:296:ASP:HA	2.02	0.40
1:B:61:LEU:HD12	1:B:61:LEU:HA	1.90	0.40
1:A:136:ASN:OD1	1:A:136:ASN:C	2.60	0.40
1:A:302:GLU:OE2	1:A:344:GLU:OE2	2.40	0.40
1:B:151:LYS:O	1:B:152:LYS:HG2	2.20	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	373/401 (93%)	351 (94%)	17 (5%)	5 (1%)	15	21
1	B	360/401 (90%)	335 (93%)	18 (5%)	7 (2%)	10	12
1	C	361/401 (90%)	343 (95%)	16 (4%)	2 (1%)	30	43
All	All	1094/1203 (91%)	1029 (94%)	51 (5%)	14 (1%)	15	21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	318	ILE
1	B	226	ASP
1	A	88	ASP
1	B	4	LYS
1	B	92	GLU
1	B	336	LEU
1	B	337	THR
1	C	337	THR
1	A	316	VAL
1	A	118	ILE
1	B	118	ILE
1	C	118	ILE
1	A	292	ILE
1	B	292	ILE

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	305/335 (91%)	284 (93%)	21 (7%)	19	30
1	B	287/335 (86%)	269 (94%)	18 (6%)	22	35
1	C	271/335 (81%)	252 (93%)	19 (7%)	19	29
All	All	863/1005 (86%)	805 (93%)	58 (7%)	20	31

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	GLN
1	A	3	ILE
1	A	6	SER
1	A	17	PHE
1	A	24	GLU
1	A	63	VAL
1	A	65	LEU
1	A	87	GLN
1	A	100	ARG
1	A	114	LYS
1	A	160	ASP
1	A	173	GLN
1	A	181	THR
1	A	196	ASP
1	A	215	TYR
1	A	218	LEU
1	A	240	THR
1	A	253	ASN
1	A	260	LEU
1	A	336	LEU
1	A	360	LEU
1	B	12	LEU
1	B	61	LEU
1	B	64	LYS
1	B	89	ASP
1	B	100	ARG
1	B	154	ASN
1	B	157	ASP
1	B	173	GLN
1	B	177	ARG
1	B	178	SER
1	B	180	LEU
1	B	181	THR
1	B	196	ASP

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Mol	Chain	Res	Type
1	B	215	TYR
1	B	241	ASP
1	B	248	ASP
1	B	253	ASN
1	B	347	ARG
1	C	6	SER
1	C	19	ARG
1	C	21	PHE
1	C	55	VAL
1	C	92	GLU
1	C	105	THR
1	C	162	GLU
1	C	181	THR
1	C	208	ASP
1	C	215	TYR
1	C	218	LEU
1	C	220	HIS
1	C	221	THR
1	C	222	LEU
1	C	253	ASN
1	C	260	LEU
1	C	335	LEU
1	C	372	MET
1	C	380	TYR

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

Mol	Chain	Res	Type
1	A	220	HIS
1	A	378	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

24 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	A	395	-	4,4,4	0.25	0	6,6,6	0.46	0
2	SO4	A	396	-	4,4,4	0.17	0	6,6,6	0.39	0
2	SO4	A	397	-	4,4,4	0.22	0	6,6,6	0.28	0
2	SO4	A	398	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	A	399	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	A	400	-	4,4,4	0.18	0	6,6,6	0.18	0
3	C8E	A	401	-	17,17,20	0.50	0	16,16,19	0.40	0
3	C8E	A	402	-	9,9,20	0.44	0	8,8,19	0.28	0
3	C8E	A	403	-	15,15,20	0.44	0	14,14,19	0.58	0
3	C8E	A	404	-	11,11,20	0.36	0	10,10,19	0.51	0
3	C8E	A	405	-	14,14,20	0.46	0	13,13,19	0.54	0
2	SO4	B	395	-	4,4,4	0.22	0	6,6,6	0.35	0
2	SO4	B	396	-	4,4,4	0.18	0	6,6,6	0.09	0
2	SO4	B	397	-	4,4,4	0.16	0	6,6,6	0.33	0
3	C8E	B	398	-	18,18,20	0.40	0	17,17,19	0.36	0
3	C8E	B	399	-	19,19,20	0.42	0	18,18,19	0.37	0
3	C8E	B	400	-	9,9,20	0.47	0	8,8,19	0.33	0
3	C8E	B	401	-	10,10,20	0.36	0	9,9,19	0.50	0
3	C8E	B	402	-	17,17,20	0.47	0	16,16,19	0.46	0
2	SO4	C	395	-	4,4,4	0.11	0	6,6,6	0.24	0
2	SO4	C	396	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	C	397	-	4,4,4	0.25	0	6,6,6	0.08	0
3	C8E	C	398	-	13,13,20	0.44	0	12,12,19	0.45	0
3	C8E	C	399	-	10,10,20	0.42	0	9,9,19	0.28	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	A	395	-	-	0/0/0/0	0/0/0/0
2	SO4	A	396	-	-	0/0/0/0	0/0/0/0
2	SO4	A	397	-	-	0/0/0/0	0/0/0/0
2	SO4	A	398	-	-	0/0/0/0	0/0/0/0
2	SO4	A	399	-	-	0/0/0/0	0/0/0/0
2	SO4	A	400	-	-	0/0/0/0	0/0/0/0
3	C8E	A	401	-	-	0/15/15/18	0/0/0/0
3	C8E	A	402	-	-	0/7/7/18	0/0/0/0
3	C8E	A	403	-	-	0/13/13/18	0/0/0/0
3	C8E	A	404	-	-	0/9/9/18	0/0/0/0
3	C8E	A	405	-	-	0/12/12/18	0/0/0/0
2	SO4	B	395	-	-	0/0/0/0	0/0/0/0
2	SO4	B	396	-	-	0/0/0/0	0/0/0/0
2	SO4	B	397	-	-	0/0/0/0	0/0/0/0
3	C8E	B	398	-	-	0/16/16/18	0/0/0/0
3	C8E	B	399	-	-	0/17/17/18	0/0/0/0
3	C8E	B	400	-	-	0/7/7/18	0/0/0/0
3	C8E	B	401	-	-	0/8/8/18	0/0/0/0
3	C8E	B	402	-	-	0/15/15/18	0/0/0/0
2	SO4	C	395	-	-	0/0/0/0	0/0/0/0
2	SO4	C	396	-	-	0/0/0/0	0/0/0/0
2	SO4	C	397	-	-	0/0/0/0	0/0/0/0
3	C8E	C	398	-	-	0/11/11/18	0/0/0/0
3	C8E	C	399	-	-	0/8/8/18	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.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	398	SO4	1	0
2	A	399	SO4	1	0
3	A	403	C8E	9	0
3	A	404	C8E	1	0
2	B	395	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	398	C8E	3	0
3	B	400	C8E	2	0
3	B	401	C8E	1	0
2	C	395	SO4	2	0
3	C	398	C8E	1	0
3	C	399	C8E	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	377/401 (94%)	0.02	5 (1%) 79 79	23, 41, 82, 118	0
1	B	368/401 (91%)	0.22	21 (5%) 27 27	22, 51, 94, 119	0
1	C	367/401 (91%)	0.39	35 (9%) 10 10	37, 69, 109, 132	0
All	All	1112/1203 (92%)	0.21	61 (5%) 29 29	22, 52, 100, 132	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	SER	6.0
1	C	26	ALA	4.9
1	C	262	TYR	4.2
1	C	242	ASP	4.1
1	C	178	SER	3.9
1	C	357	SER	3.9
1	C	258	TYR	3.9
1	C	260	LEU	3.8
1	C	316	VAL	3.7
1	B	359	PRO	3.6
1	C	394	TRP	3.6
1	C	226	ASP	3.5
1	A	359	PRO	3.5
1	B	34	TRP	3.4
1	C	34	TRP	3.3
1	C	363	LEU	3.2
1	C	223	PRO	3.2
1	B	380	TYR	3.2
1	C	31	ALA	3.2
1	B	226	ASP	3.1
1	C	16	TYR	3.1
1	C	224	ILE	3.1
1	C	89	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	210	PHE	3.0
1	C	311	TYR	3.0
1	B	45	GLY	2.9
1	C	259	SER	2.8
1	B	316	VAL	2.8
1	A	317	GLY	2.8
1	B	91	GLY	2.8
1	C	265	PHE	2.8
1	B	315	GLY	2.7
1	B	317	GLY	2.7
1	C	227	LYS	2.7
1	B	28	GLN	2.7
1	B	358	GLY	2.6
1	C	358	GLY	2.6
1	C	263	HIS	2.6
1	B	225	ALA	2.6
1	C	27	SER	2.5
1	B	5	ASP	2.5
1	C	3	ILE	2.5
1	B	22	ARG	2.5
1	C	208	ASP	2.5
1	A	226	ASP	2.3
1	A	318	ILE	2.3
1	C	173	GLN	2.3
1	C	29	SER	2.3
1	C	163	ASP	2.2
1	A	225	ALA	2.2
1	B	3	ILE	2.2
1	C	158	SER	2.2
1	B	357	SER	2.2
1	B	394	TRP	2.2
1	B	263	HIS	2.2
1	C	222	LEU	2.1
1	C	337	THR	2.1
1	C	42	TYR	2.1
1	C	317	GLY	2.1
1	B	65	LEU	2.0
1	B	314	ALA	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
3	C8E	C	399	11/21	0.84	0.27	10.04	62,68,73,74	0
2	SO4	A	400	5/5	0.78	0.24	4.60	110,114,116,119	0
3	C8E	A	401	18/21	0.86	0.20	3.02	47,63,72,74	0
2	SO4	B	396	5/5	0.81	0.20	2.97	103,108,110,114	0
3	C8E	B	402	18/21	0.87	0.19	2.36	38,59,74,78	0
3	C8E	A	403	16/21	0.77	0.23	2.35	68,83,88,89	0
3	C8E	A	404	12/21	0.78	0.21	2.16	61,78,83,83	0
3	C8E	C	398	14/21	0.86	0.20	2.15	58,65,75,75	0
3	C8E	B	399	20/21	0.82	0.20	2.07	54,67,81,81	0
2	SO4	B	397	5/5	0.91	0.17	1.34	65,70,74,86	0
3	C8E	A	405	15/21	0.83	0.17	1.24	62,72,87,89	0
2	SO4	B	395	5/5	0.92	0.21	1.17	49,68,74,76	0
2	SO4	C	396	5/5	0.85	0.30	0.80	118,120,122,126	0
3	C8E	B	400	10/21	0.81	0.19	0.49	58,68,78,79	0
2	SO4	A	398	5/5	0.86	0.18	0.27	108,109,110,114	0
2	SO4	C	397	5/5	0.92	0.19	0.16	100,101,103,104	0
2	SO4	A	395	5/5	0.97	0.18	0.01	51,62,69,77	0
3	C8E	B	401	11/21	0.91	0.14	-0.03	41,53,76,77	0
3	C8E	B	398	19/21	0.90	0.15	-0.24	46,60,67,70	0
2	SO4	A	397	5/5	0.95	0.15	-0.68	57,59,60,65	0
2	SO4	A	399	5/5	0.94	0.10	-1.15	67,74,78,86	0
2	SO4	C	395	5/5	0.97	0.12	-2.05	61,63,67,68	0
3	C8E	A	402	10/21	0.71	0.20	-	94,97,98,99	0
2	SO4	A	396	5/5	0.96	0.16	-	56,57,65,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.