



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:12 AM UTC

PDB ID : 1EXZ / pdb_00001exz
Title : STRUCTURE OF STEM CELL FACTOR
Authors : Zhang, Z.; Zhang, R.; Joachimiak, A.; Schlessinger, J.; Kong, X.
Deposited on : 2000-05-05
Resolution : 2.30 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

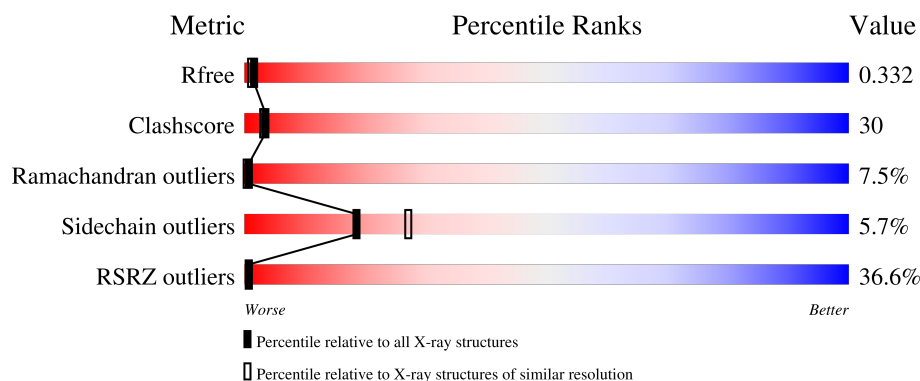
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	141	35% 38% 49% 7% 6%
1	B	141	38% 50% 43% 6%
1	C	141	32% 56% 27% 9% 7%
1	D	141	33% 44% 35% 9% 12%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4236 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 STEM CELL FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	133	Total	C	N	O	S	0	0	0
			1049	672	166	204	7			
1	B	140	Total	C	N	O	S	0	0	0
			1072	682	175	208	7			
1	C	131	Total	C	N	O	S	0	0	0
			998	638	157	197	6			
1	D	124	Total	C	N	O	S	0	0	0
			971	622	153	191	5			

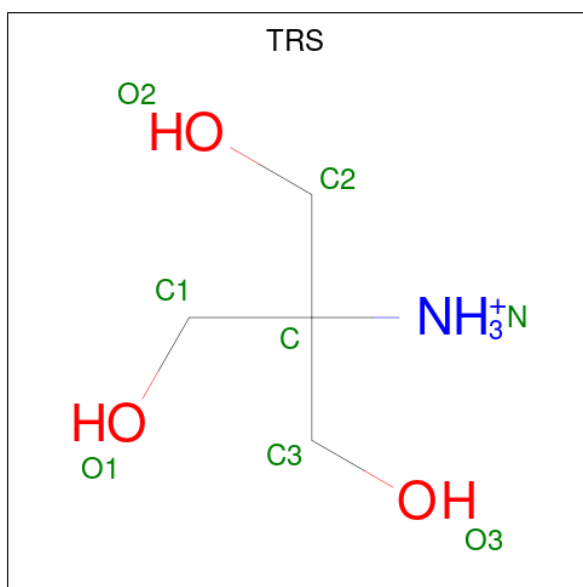
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SAMARIUM (III) ION (CCD ID: SM) (formula: Sm).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Sm	0	0
			2	2		
3	C	2	Total	Sm	0	0
			2	2		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			8	4	1	3		

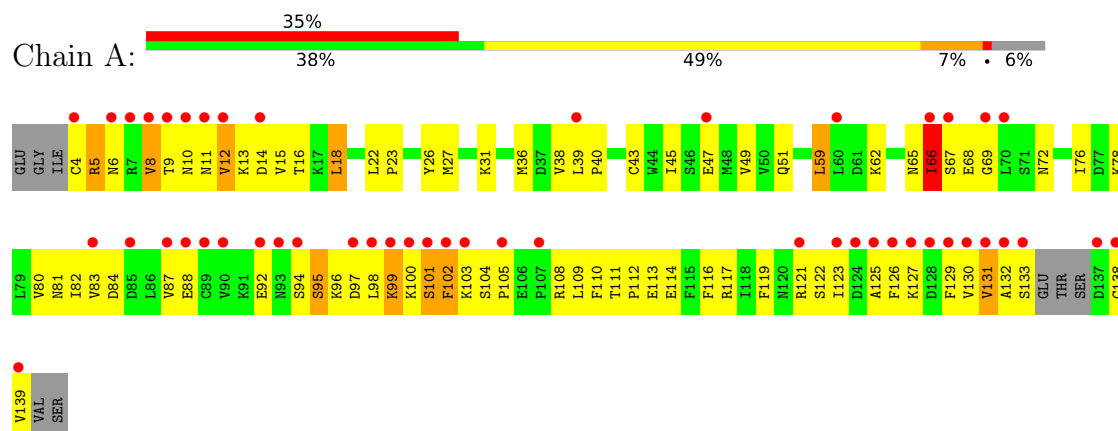
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	32	Total	O	0	0
			32	32		
5	C	37	Total	O	0	0
			37	37		
5	D	28	Total	O	0	0
			28	28		

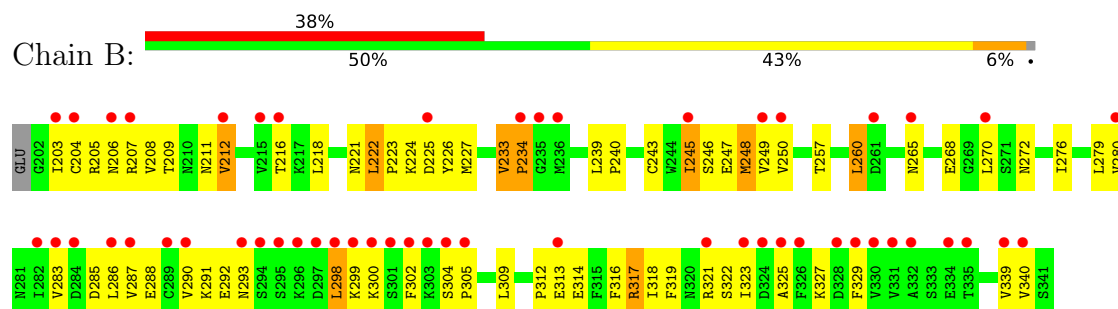
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 ($RSRZ > 2$). 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.

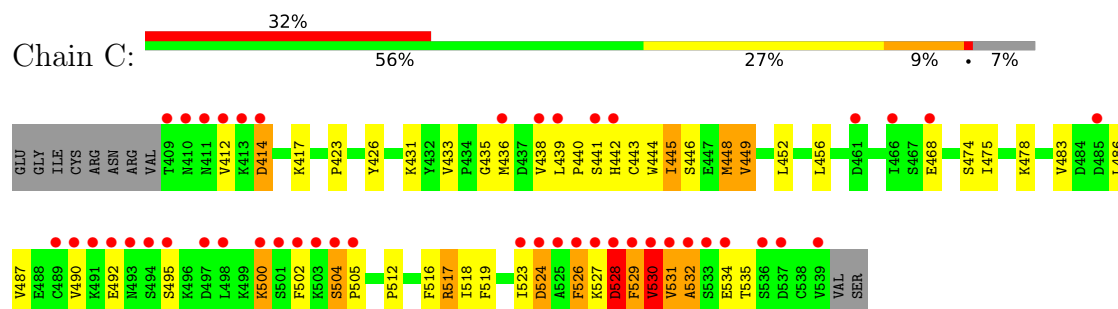
• Molecule 1: STEM CELL FACTOR



• Molecule 1: STEM CELL FACTOR

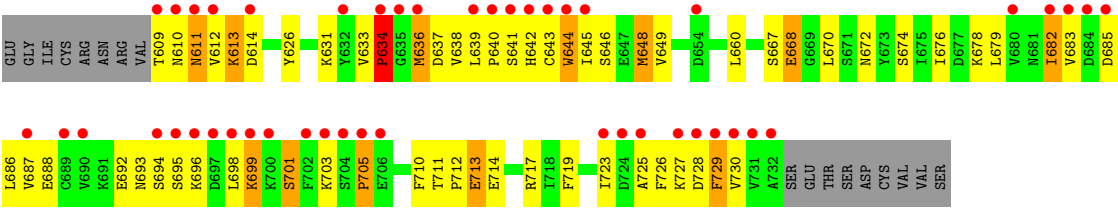


• Molecule 1: STEM CELL FACTOR



• Molecule 1: STEM CELL FACTOR





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.15Å 87.53Å 79.43Å 90.00° 97.76° 90.00°	Depositor
Resolution (Å)	40.00 – 2.30 40.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	10.0 (40.00-2.30) 98.0 (40.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.294 0.295 , 0.332	Depositor DCC
R_{free} test set	1071 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4236	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% 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: SM, TRS, CA

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	0.42	0/1067	0.91	2/1444 (0.1%)
1	B	0.40	0/1090	0.91	4/1483 (0.3%)
1	C	0.45	0/1016	0.96	7/1385 (0.5%)
1	D	0.40	0/988	0.88	2/1342 (0.1%)
All	All	0.42	0/4161	0.92	15/5654 (0.3%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	ILE	N-CA-C	7.98	119.72	110.62
1	C	414	ASP	N-CA-C	-7.87	102.78	111.36
1	D	717	ARG	N-CA-C	-7.51	103.10	111.82
1	C	445	ILE	N-CA-C	6.87	118.45	110.62
1	B	317	ARG	N-CA-C	-6.76	103.15	111.40
1	A	117	ARG	N-CA-C	-6.68	103.47	111.69
1	C	444	TRP	N-CA-C	6.57	122.11	114.62
1	B	233	VAL	CA-C-N	6.51	127.98	119.84
1	B	233	VAL	C-N-CA	6.51	127.98	119.84
1	A	131	VAL	N-CA-C	6.46	113.12	106.21
1	C	526	PHE	N-CA-C	-5.79	106.56	113.97
1	C	528	ASP	N-CA-C	5.76	123.06	110.80
1	C	517	ARG	N-CA-C	-5.63	105.29	111.82
1	C	530	VAL	N-CA-C	5.17	120.10	109.34
1	D	711	THR	N-CA-C	-5.09	102.64	110.07

There are no chirality outliers.

There are no planarity outliers.

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	A	1049	0	1042	85	1
1	B	1072	0	1033	60	0
1	C	998	0	948	50	0
1	D	971	0	949	55	1
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	B	2	0	0	0	1
3	C	2	0	0	0	1
4	D	8	0	11	0	0
5	A	35	0	0	2	0
5	B	32	0	0	1	0
5	C	37	0	0	2	0
5	D	28	0	0	1	0
All	All	4236	0	3983	242	2

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 30.

All (242) 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:531:VAL:HG12	1:C:532:ALA:H	1.12	1.15
1:C:423:PRO:HG2	1:C:426:TYR:HB2	1.48	0.94
1:A:65:ASN:HD22	1:A:66:ILE:H	1.16	0.93
1:C:452:LEU:O	1:C:456:LEU:HD23	1.72	0.90
1:C:436:MET:HE2	1:C:518:ILE:HG23	1.52	0.89
1:C:527:LYS:HG3	1:C:528:ASP:H	1.38	0.89
1:B:223:PRO:HG2	1:B:226:TYR:HB2	1.56	0.88
1:A:111:THR:HG23	1:A:114:GLU:H	1.40	0.85
1:B:206:ASN:O	1:B:207:ARG:HG2	1.77	0.85
1:C:529:PHE:HD1	1:C:530:VAL:H	1.23	0.83
1:C:438:VAL:HG23	1:C:439:LEU:HD12	1.59	0.83
1:C:531:VAL:HG12	1:C:532:ALA:N	1.93	0.81
1:C:504:SER:H	1:C:505:PRO:CD	1.95	0.79
1:D:638:VAL:HG23	1:D:639:LEU:HD12	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:CYS:O	1:B:208:VAL:HG21	1.85	0.75
1:C:531:VAL:CG1	1:C:532:ALA:H	1.94	0.75
1:A:13:LYS:HG3	1:A:14:ASP:H	1.53	0.74
1:A:31:LYS:HB3	1:A:105:PRO:HG2	1.71	0.73
1:A:23:PRO:HG2	1:A:26:TYR:HB2	1.70	0.72
1:A:65:ASN:O	1:A:66:ILE:HG23	1.89	0.72
1:C:532:ALA:HB1	1:C:535:THR:HB	1.69	0.72
1:C:504:SER:H	1:C:505:PRO:HD3	1.53	0.72
1:D:643:CYS:HB3	1:D:701:SER:CB	2.20	0.72
1:B:206:ASN:O	1:B:208:VAL:HG23	1.91	0.71
1:D:641:SER:HB2	1:D:645:ILE:HD11	1.72	0.70
1:A:95:SER:C	1:A:97:ASP:H	1.99	0.70
1:D:633:VAL:HG13	1:D:634:PRO:HD2	1.74	0.70
1:B:233:VAL:HG23	1:B:248:MET:HE3	1.74	0.69
1:A:100:LYS:HA	5:A:915:HOH:O	1.92	0.69
1:B:313:GLU:OE2	1:B:314:GLU:HG3	1.93	0.69
1:B:233:VAL:HG23	1:B:248:MET:CE	2.24	0.68
1:D:648:MET:HE2	1:D:648:MET:HA	1.76	0.68
1:B:314:GLU:O	1:B:318:ILE:HD13	1.94	0.67
1:B:248:MET:HE2	1:B:248:MET:HA	1.76	0.67
1:A:47:GLU:OE2	1:A:103:LYS:HG3	1.95	0.67
1:C:445:ILE:HD12	1:C:446:SER:N	2.09	0.67
1:D:729:PHE:CD2	1:D:730:VAL:HG23	2.29	0.66
1:D:613:LYS:HB2	1:D:613:LYS:NZ	2.11	0.66
1:C:431:LYS:HB3	1:C:505:PRO:HG2	1.78	0.66
1:D:641:SER:HB2	1:D:645:ILE:CD1	2.26	0.65
1:A:96:LYS:HB3	1:A:133:SER:H	1.62	0.65
1:B:208:VAL:HG12	1:B:208:VAL:O	1.97	0.64
1:B:205:ARG:HA	1:B:208:VAL:HB	1.80	0.63
1:A:65:ASN:HD22	1:A:66:ILE:N	1.91	0.63
1:B:212:VAL:O	1:B:216:THR:HG23	1.98	0.63
1:D:649:VAL:HG12	1:D:687:VAL:HG22	1.80	0.62
1:A:65:ASN:ND2	1:A:66:ILE:H	1.91	0.62
1:C:445:ILE:HD12	1:C:446:SER:H	1.63	0.62
1:B:226:TYR:O	1:B:312:PRO:HD3	2.00	0.62
1:A:100:LYS:HE3	1:A:103:LYS:NZ	2.15	0.61
1:A:38:VAL:HG23	1:A:39:LEU:CD1	2.30	0.61
1:B:227:MET:HG3	1:B:309:LEU:HB3	1.82	0.61
1:B:283:VAL:HG21	1:B:319:PHE:HE1	1.65	0.61
1:A:99:LYS:O	1:A:99:LYS:HG3	1.99	0.61
1:C:426:TYR:O	1:C:512:PRO:HD3	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:645:ILE:HD11	1:D:725:ALA:HB1	1.82	0.60
1:D:679:LEU:O	1:D:682:ILE:HD13	2.01	0.60
1:D:631:LYS:HB3	1:D:705:PRO:HB2	1.82	0.60
1:D:682:ILE:HD13	1:D:683:VAL:N	2.16	0.60
1:A:78:LYS:NZ	1:A:82:ILE:HD11	2.17	0.59
1:B:279:LEU:O	1:B:283:VAL:HG23	2.02	0.59
1:A:12:VAL:HA	1:A:15:VAL:HB	1.85	0.59
1:D:633:VAL:HG11	1:D:644:TRP:HB3	1.84	0.59
1:C:449:VAL:HG12	1:C:487:VAL:HG22	1.84	0.59
1:A:12:VAL:HG12	1:A:16:THR:OG1	2.03	0.59
1:D:633:VAL:H	1:D:648:MET:HE3	1.67	0.59
1:A:94:SER:HB2	1:A:99:LYS:HB3	1.84	0.58
1:C:504:SER:N	1:C:505:PRO:CD	2.66	0.58
1:B:209:THR:HG22	1:B:211:ASN:ND2	2.18	0.58
1:A:13:LYS:HG3	1:A:14:ASP:N	2.18	0.58
1:C:448:MET:HA	1:C:448:MET:HE3	1.85	0.58
1:A:127:LYS:HG3	1:C:531:VAL:HA	1.86	0.58
1:C:440:PRO:HG2	1:C:443:CYS:SG	2.44	0.58
1:C:500:LYS:C	1:C:502:PHE:H	2.11	0.58
1:D:686:LEU:HD22	1:D:726:PHE:CD2	2.38	0.57
1:A:47:GLU:CD	1:A:103:LYS:HA	2.30	0.56
1:C:448:MET:HA	1:C:448:MET:CE	2.36	0.56
1:B:203:ILE:O	1:B:205:ARG:HG2	2.05	0.56
1:A:125:ALA:O	1:A:129:PHE:HB2	2.06	0.56
1:B:249:VAL:HG12	1:B:287:VAL:HG22	1.88	0.56
1:A:100:LYS:HE3	1:A:103:LYS:HZ1	1.70	0.56
1:D:683:VAL:O	1:D:687:VAL:HG23	2.06	0.56
1:D:698:LEU:HG	1:D:699:LYS:H	1.71	0.56
1:C:527:LYS:HG3	1:C:528:ASP:N	2.16	0.56
1:D:730:VAL:HG12	1:D:730:VAL:O	2.06	0.56
1:B:317:ARG:HB3	1:B:321:ARG:NH2	2.21	0.55
1:C:486:LEU:O	1:C:490:VAL:HG23	2.05	0.55
1:B:247:GLU:OE1	1:B:305:PRO:HD3	2.06	0.55
1:A:8:VAL:O	1:A:8:VAL:HG12	2.06	0.55
1:D:674:SER:O	1:D:678:LYS:HG2	2.07	0.55
1:A:100:LYS:O	1:A:101:SER:CB	2.54	0.55
1:D:678:LYS:O	1:D:682:ILE:HG23	2.07	0.55
1:D:726:PHE:C	1:D:728:ASP:H	2.15	0.54
1:A:4:CYS:O	1:A:5:ARG:C	2.50	0.54
1:B:283:VAL:CG2	1:B:319:PHE:HE1	2.20	0.54
1:A:38:VAL:HG23	1:A:39:LEU:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ILE:O	1:B:280:VAL:HG23	2.07	0.53
1:C:441:SER:O	1:C:445:ILE:HG13	2.08	0.53
1:D:609:THR:HG23	1:D:727:LYS:NZ	2.22	0.53
1:A:119:PHE:CE2	1:A:123:ILE:HD12	2.43	0.53
1:D:626:TYR:O	1:D:712:PRO:HD3	2.09	0.53
1:A:95:SER:C	1:A:97:ASP:N	2.64	0.53
1:A:23:PRO:HG2	1:A:26:TYR:CB	2.39	0.53
1:A:59:LEU:CD1	1:A:76:ILE:HD13	2.39	0.53
1:A:94:SER:CB	1:A:99:LYS:HB3	2.39	0.53
1:D:644:TRP:H	1:D:644:TRP:CD1	2.27	0.52
1:D:609:THR:OG1	1:D:727:LYS:HE2	2.09	0.52
1:A:10:ASN:CB	1:A:82:ILE:HD13	2.40	0.52
1:B:203:ILE:O	1:B:204:CYS:C	2.52	0.52
1:C:483:VAL:O	1:C:487:VAL:HG23	2.10	0.52
1:A:40:PRO:HG2	1:A:43:CYS:SG	2.49	0.52
1:C:474:SER:O	1:C:478:LYS:HG2	2.10	0.51
1:A:122:SER:O	1:A:125:ALA:HB3	2.11	0.51
1:A:11:ASN:C	1:A:13:LYS:H	2.19	0.50
1:B:339:VAL:HG12	1:B:340:VAL:N	2.27	0.50
1:A:47:GLU:OE2	1:A:103:LYS:HA	2.10	0.50
1:B:322:SER:O	1:B:325:ALA:HB3	2.11	0.50
1:A:138:CYS:O	1:A:139:VAL:HB	2.11	0.50
1:B:205:ARG:HH21	1:B:327:LYS:HB2	1.77	0.50
1:C:436:MET:CE	1:C:518:ILE:HG23	2.34	0.50
1:A:81:ASN:ND2	5:A:947:HOH:O	2.44	0.50
1:A:111:THR:HG22	1:A:114:GLU:CD	2.36	0.50
1:D:719:PHE:O	1:D:723:ILE:HG12	2.12	0.49
1:A:83:VAL:O	1:A:87:VAL:HG23	2.13	0.49
1:A:108:ARG:HG3	1:A:110:PHE:CE1	2.48	0.49
1:D:686:LEU:HB3	1:D:726:PHE:CE2	2.47	0.49
1:D:638:VAL:HG23	1:D:639:LEU:N	2.27	0.49
1:A:38:VAL:HG23	1:A:39:LEU:HD13	1.95	0.49
1:C:435:GLY:CA	1:C:439:LEU:HD13	2.43	0.49
1:D:698:LEU:HG	1:D:699:LYS:N	2.27	0.49
1:C:524:ASP:C	1:C:526:PHE:H	2.20	0.49
1:D:693:ASN:C	1:D:695:SER:H	2.19	0.49
1:B:206:ASN:C	1:B:207:ARG:HG2	2.37	0.48
1:B:209:THR:HG22	1:B:211:ASN:CG	2.39	0.48
1:D:644:TRP:O	1:D:646:SER:N	2.45	0.48
1:A:66:ILE:O	1:A:68:GLU:N	2.47	0.48
1:A:27:MET:HE3	1:A:109:LEU:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:PRO:HG2	1:B:243:CYS:SG	2.53	0.48
1:C:478:LYS:HE2	5:C:909:HOH:O	2.13	0.48
1:A:65:ASN:C	1:A:66:ILE:HG12	2.38	0.48
1:C:442:HIS:CD2	1:C:534:GLU:HA	2.49	0.47
1:D:637:ASP:OD1	1:D:638:VAL:HG13	2.13	0.47
1:B:265:ASN:OD1	1:B:265:ASN:O	2.32	0.47
1:A:100:LYS:HG2	1:A:101:SER:H	1.80	0.47
1:B:268:GLU:HG3	1:C:517:ARG:CZ	2.44	0.47
1:B:206:ASN:C	1:B:208:VAL:HG23	2.40	0.47
1:B:260:LEU:HD12	1:B:260:LEU:HA	1.79	0.47
1:C:449:VAL:CG1	1:C:487:VAL:HG22	2.45	0.47
1:D:713:GLU:HB2	5:D:838:HOH:O	2.15	0.47
1:B:317:ARG:HB3	1:B:321:ARG:CZ	2.45	0.46
1:A:4:CYS:O	1:A:6:ASN:N	2.48	0.46
1:D:692:GLU:C	1:D:694:SER:H	2.23	0.46
1:C:414:ASP:HB3	1:C:475:ILE:HG23	1.97	0.46
1:A:100:LYS:O	1:A:101:SER:HB3	2.14	0.46
1:D:648:MET:HA	1:D:648:MET:CE	2.45	0.46
1:A:126:PHE:O	1:A:127:LYS:C	2.59	0.46
1:B:246:SER:O	1:B:250:VAL:HG23	2.15	0.46
1:D:609:THR:HG23	1:D:727:LYS:HZ3	1.79	0.46
1:D:679:LEU:HA	1:D:682:ILE:HD12	1.96	0.46
1:A:36:MET:O	1:A:36:MET:HG2	2.15	0.46
1:D:633:VAL:N	1:D:648:MET:HE3	2.30	0.46
1:B:329:PHE:C	1:B:329:PHE:CD2	2.94	0.45
1:A:45:ILE:HD11	1:A:126:PHE:CE1	2.51	0.45
1:D:638:VAL:HG23	1:D:639:LEU:CD1	2.40	0.45
1:A:111:THR:HG22	1:A:114:GLU:CG	2.46	0.45
1:D:640:PRO:C	1:D:642:HIS:H	2.23	0.45
1:C:529:PHE:HD1	1:C:530:VAL:N	2.02	0.45
1:A:97:ASP:O	1:A:99:LYS:N	2.47	0.45
1:B:211:ASN:ND2	5:B:939:HOH:O	2.49	0.45
1:B:223:PRO:C	1:B:225:ASP:H	2.24	0.45
1:B:218:LEU:HG	1:B:222:LEU:HD22	1.98	0.45
1:C:486:LEU:HD22	1:C:526:PHE:CZ	2.52	0.45
1:A:18:LEU:HD13	1:A:116:PHE:CZ	2.51	0.45
1:A:18:LEU:HD22	1:A:22:LEU:CD1	2.47	0.45
1:A:80:VAL:O	1:A:83:VAL:HG12	2.17	0.45
1:B:206:ASN:O	1:B:207:ARG:CG	2.59	0.44
1:B:223:PRO:C	1:B:225:ASP:N	2.74	0.44
1:B:287:VAL:HG12	1:B:287:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:C	1:A:68:GLU:H	2.24	0.44
1:A:127:LYS:NZ	1:C:531:VAL:HG13	2.32	0.44
1:B:318:ILE:HD12	1:B:321:ARG:NH1	2.32	0.44
1:D:667:SER:C	1:D:668:GLU:HG3	2.43	0.44
1:B:316:PHE:HA	1:B:319:PHE:HB3	2.00	0.44
1:D:679:LEU:O	1:D:683:VAL:HG12	2.17	0.44
1:A:119:PHE:CZ	1:A:123:ILE:HD12	2.53	0.44
1:C:532:ALA:HB1	1:C:535:THR:CB	2.44	0.44
1:D:636:MET:HA	1:D:644:TRP:CD1	2.52	0.44
1:A:119:PHE:CD2	1:A:119:PHE:C	2.96	0.43
1:A:45:ILE:HD11	1:A:126:PHE:CD1	2.53	0.43
1:B:283:VAL:CG2	1:B:319:PHE:CE1	3.01	0.43
1:A:84:ASP:O	1:A:87:VAL:HB	2.18	0.43
1:D:613:LYS:HB2	1:D:613:LYS:HZ3	1.81	0.43
1:B:319:PHE:CZ	1:B:323:ILE:HD11	2.53	0.43
1:A:78:LYS:HZ3	1:A:82:ILE:HD11	1.83	0.43
1:A:26:TYR:O	1:A:112:PRO:HD3	2.18	0.43
1:B:204:CYS:O	1:B:204:CYS:SG	2.76	0.43
1:B:257:THR:O	1:B:260:LEU:HB2	2.19	0.43
1:B:292:GLU:O	1:B:293:ASN:C	2.62	0.43
1:A:101:SER:O	1:A:102:PHE:CB	2.66	0.43
1:A:111:THR:CG2	1:A:114:GLU:H	2.20	0.43
1:A:121:ARG:HG3	1:C:529:PHE:CD2	2.54	0.43
1:A:121:ARG:HG3	1:C:529:PHE:HD2	1.84	0.43
1:A:116:PHE:HA	1:A:119:PHE:HB3	2.01	0.43
1:C:516:PHE:HA	1:C:519:PHE:HB3	2.00	0.43
1:D:686:LEU:HD22	1:D:726:PHE:HD2	1.80	0.43
1:A:47:GLU:OE2	1:A:51:GLN:NE2	2.44	0.42
1:A:88:GLU:O	1:A:92:GLU:HG3	2.19	0.42
1:B:288:GLU:C	1:B:290:VAL:N	2.76	0.42
1:C:433:VAL:HG23	1:C:448:MET:HE3	2.00	0.42
1:A:127:LYS:HD2	1:C:531:VAL:HG13	2.01	0.42
1:B:304:SER:HA	1:B:305:PRO:HD3	1.91	0.42
1:D:660:LEU:HD13	1:D:676:ILE:HG22	2.01	0.42
1:A:95:SER:O	1:A:96:LYS:HB2	2.19	0.42
1:A:127:LYS:CE	1:C:531:VAL:HG13	2.50	0.42
1:B:209:THR:O	1:B:211:ASN:ND2	2.52	0.42
1:A:72:ASN:O	1:A:76:ILE:HG13	2.20	0.42
1:D:613:LYS:HB2	1:D:613:LYS:HZ2	1.84	0.42
1:A:130:VAL:HG23	1:A:131:VAL:N	2.35	0.42
1:B:206:ASN:C	1:B:208:VAL:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LEU:O	1:B:300:LYS:N	2.49	0.42
1:B:221:ASN:HD22	1:B:272:ASN:CG	2.28	0.42
1:B:286:LEU:C	1:B:288:GLU:N	2.76	0.42
1:D:638:VAL:HG23	1:D:639:LEU:H	1.84	0.42
1:A:102:PHE:O	1:A:103:LYS:HB3	2.19	0.42
1:D:639:LEU:HB3	1:D:640:PRO:HD2	2.01	0.42
1:A:62:LYS:O	1:B:224:LYS:HG3	2.20	0.42
1:C:468:GLU:HB3	5:C:925:HOH:O	2.20	0.42
1:A:11:ASN:C	1:A:13:LYS:N	2.78	0.41
1:D:672:ASN:O	1:D:676:ILE:HG13	2.19	0.41
1:A:111:THR:HG22	1:A:114:GLU:HB2	2.02	0.41
1:D:685:ASP:O	1:D:688:GLU:HB3	2.21	0.41
1:A:13:LYS:HG3	1:A:14:ASP:OD1	2.20	0.41
1:C:486:LEU:HD22	1:C:526:PHE:CE2	2.55	0.41
1:B:285:ASP:O	1:B:288:GLU:HB2	2.21	0.41
1:D:611:ASN:HB3	1:D:614:ASP:HB2	2.03	0.41
1:A:111:THR:HG22	1:A:114:GLU:OE2	2.21	0.41
1:B:286:LEU:C	1:B:288:GLU:H	2.28	0.41
1:D:710:PHE:HB3	1:D:714:GLU:HG3	2.03	0.41
1:D:641:SER:HB2	1:D:645:ILE:HD12	2.03	0.40
1:A:130:VAL:HG23	1:A:131:VAL:HG13	2.03	0.40
1:C:528:ASP:HB3	1:C:529:PHE:CD1	2.56	0.40
1:C:527:LYS:HG3	1:C:528:ASP:OD1	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:713:GLU:OE1	3:B:803:SM:SM[2_645]	2.12	0.08
1:A:88:GLU:OE2	3:C:801:SM:SM[2_656]	2.17	0.03

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	129/141 (92%)	103 (80%)	13 (10%)	13 (10%)	0	0
1	B	138/141 (98%)	113 (82%)	20 (14%)	5 (4%)	2	1
1	C	129/141 (92%)	105 (81%)	15 (12%)	9 (7%)	1	0
1	D	121/141 (86%)	98 (81%)	11 (9%)	12 (10%)	0	0
All	All	517/564 (92%)	419 (81%)	59 (11%)	39 (8%)	1	0

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	66	ILE
1	A	67	SER
1	A	132	ALA
1	B	291	LYS
1	B	298	LEU
1	C	492	GLU
1	C	495	SER
1	C	500	LYS
1	C	504	SER
1	C	530	VAL
1	C	531	VAL
1	D	634	PRO
1	D	701	SER
1	A	9	THR
1	A	95	SER
1	A	101	SER
1	C	532	ALA
1	D	611	ASN
1	D	612	VAL
1	D	696	LYS
1	D	699	LYS
1	D	703	LYS
1	D	729	PHE
1	A	69	GLY
1	A	99	LYS
1	A	102	PHE
1	B	299	LYS
1	C	528	ASP
1	D	610	ASN
1	B	234	PRO

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Mol	Chain	Res	Type
1	C	412	VAL
1	D	636	MET
1	D	644	TRP
1	A	98	LEU
1	B	302	PHE
1	D	705	PRO
1	A	8	VAL
1	A	104	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	125/135 (93%)	119 (95%)	6 (5%)	23	35
1	B	121/135 (90%)	113 (93%)	8 (7%)	15	21
1	C	112/135 (83%)	106 (95%)	6 (5%)	20	29
1	D	113/135 (84%)	106 (94%)	7 (6%)	16	24
All	All	471/540 (87%)	444 (94%)	27 (6%)	18	27

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	18	LEU
1	A	49	VAL
1	A	59	LEU
1	A	66	ILE
1	A	113	GLU
1	B	212	VAL
1	B	222	LEU
1	B	234	PRO
1	B	239	LEU
1	B	245	ILE
1	B	248	MET
1	B	260	LEU

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Mol	Chain	Res	Type
1	B	270	LEU
1	C	417	LYS
1	C	448	MET
1	C	449	VAL
1	C	523	ILE
1	C	524	ASP
1	C	529	PHE
1	D	613	LYS
1	D	634	PRO
1	D	648	MET
1	D	668	GLU
1	D	670	LEU
1	D	682	ILE
1	D	713	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	81	ASN
1	A	120	ASN
1	B	210	ASN
1	B	211	ASN
1	B	221	ASN
1	B	242	HIS
1	C	442	HIS
1	C	472	ASN
1	C	520	ASN
1	D	611	ASN
1	D	642	HIS
1	D	665	ASN
1	D	720	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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
4	TRS	D	807	-	7,7,7	1.84	1 (14%)	9,9,9	1.49	1 (11%)

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
4	TRS	D	807	-	-	1/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	807	TRS	C2-C	-4.32	1.41	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	807	TRS	O2-C2-C	2.86	118.85	110.88

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	807	TRS	C3-C-C2-O2

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	731:VAL	C	732:ALA	N	8.59

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	133/141 (94%)	1.71	49 (36%) 1 1	18, 41, 88, 109	0
1	B	140/141 (99%)	1.83	53 (37%) 1 0	21, 48, 100, 104	0
1	C	131/141 (92%)	1.71	45 (34%) 1 1	18, 37, 92, 119	0
1	D	124/141 (87%)	1.86	46 (37%) 1 1	19, 47, 105, 114	0
All	All	528/564 (93%)	1.78	193 (36%) 1 1	18, 45, 99, 119	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	412	VAL	7.2
1	C	501	SER	6.7
1	D	641	SER	6.4
1	A	10	ASN	6.1
1	A	89	CYS	5.9
1	B	302	PHE	5.9
1	B	301	SER	5.8
1	D	683	VAL	5.8
1	B	295	SER	5.6
1	C	502	PHE	5.6
1	D	732	ALA	5.4
1	A	8	VAL	5.4
1	D	612	VAL	5.4
1	C	410	ASN	5.3
1	C	529	PHE	5.3
1	B	331	VAL	5.1
1	D	640	PRO	5.0
1	C	525	ALA	5.0
1	D	731	VAL	4.9
1	A	7	ARG	4.6
1	C	530	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	536	SER	4.5
1	A	97	ASP	4.5
1	A	66	ILE	4.5
1	C	494	SER	4.4
1	B	284	ASP	4.4
1	A	131	VAL	4.4
1	D	682	ILE	4.4
1	A	67	SER	4.4
1	A	69	GLY	4.3
1	B	294	SER	4.3
1	B	332	ALA	4.3
1	B	330	VAL	4.2
1	D	642	HIS	4.2
1	D	635	GLY	4.2
1	B	305	PRO	4.2
1	A	70	LEU	4.1
1	D	730	VAL	4.1
1	D	705	PRO	4.1
1	A	125	ALA	4.1
1	D	644	TRP	4.1
1	A	128	ASP	4.1
1	A	101	SER	4.1
1	D	654	ASP	4.0
1	A	132	ALA	4.0
1	C	539	VAL	4.0
1	D	729	PHE	4.0
1	C	531	VAL	3.9
1	D	636	MET	3.9
1	C	409	THR	3.9
1	C	413	LYS	3.9
1	A	133	SER	3.8
1	A	100	LYS	3.8
1	B	207	ARG	3.8
1	D	645	ILE	3.8
1	B	290	VAL	3.8
1	C	489	CYS	3.8
1	A	90	VAL	3.8
1	C	495	SER	3.7
1	B	206	ASN	3.7
1	D	687	VAL	3.7
1	C	505	PRO	3.6
1	B	326	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	98	LEU	3.6
1	C	498	LEU	3.6
1	D	690	VAL	3.6
1	D	725	ALA	3.6
1	B	293	ASN	3.5
1	B	289	CYS	3.5
1	A	130	VAL	3.5
1	A	102	PHE	3.5
1	C	493	ASN	3.5
1	C	526	PHE	3.5
1	B	298	LEU	3.5
1	D	706	GLU	3.5
1	A	93	ASN	3.4
1	D	680	VAL	3.4
1	C	528	ASP	3.4
1	B	212	VAL	3.4
1	A	11	ASN	3.4
1	D	698	LEU	3.3
1	D	684	ASP	3.3
1	D	609	THR	3.3
1	D	728	ASP	3.2
1	C	500	LYS	3.2
1	C	532	ALA	3.2
1	B	297	ASP	3.2
1	A	127	LYS	3.2
1	B	225	ASP	3.2
1	C	414	ASP	3.2
1	C	441	SER	3.1
1	A	9	THR	3.1
1	B	283	VAL	3.1
1	D	704	SER	3.1
1	A	129	PHE	3.1
1	A	85	ASP	3.1
1	C	439	LEU	3.1
1	B	300	LYS	3.0
1	B	287	VAL	3.0
1	B	340	VAL	3.0
1	B	323	ILE	3.0
1	C	504	SER	3.0
1	C	411	ASN	3.0
1	C	497	ASP	3.0
1	C	438	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	99	LYS	2.9
1	B	234	PRO	2.9
1	D	634	PRO	2.9
1	B	339	VAL	2.9
1	D	727	LYS	2.9
1	A	139	VAL	2.9
1	B	329	PHE	2.8
1	D	702	PHE	2.8
1	A	12	VAL	2.8
1	B	324	ASP	2.8
1	A	92	GLU	2.8
1	B	249	VAL	2.8
1	A	126	PHE	2.8
1	B	236	MET	2.8
1	A	4	CYS	2.8
1	B	328	ASP	2.7
1	A	137	ASP	2.7
1	D	697	ASP	2.7
1	C	491	LYS	2.7
1	C	492	GLU	2.7
1	D	689	CYS	2.7
1	B	335	THR	2.7
1	D	723	ILE	2.7
1	B	286	LEU	2.7
1	D	703	LYS	2.6
1	B	321	ARG	2.6
1	C	533	SER	2.6
1	B	204	CYS	2.6
1	A	88	GLU	2.6
1	B	304	SER	2.6
1	A	138	CYS	2.6
1	B	325	ALA	2.6
1	A	6	ASN	2.6
1	B	303	LYS	2.6
1	A	14	ASP	2.5
1	C	436	MET	2.5
1	D	611	ASN	2.5
1	C	490	VAL	2.5
1	B	299	LYS	2.5
1	A	94	SER	2.5
1	B	270	LEU	2.5
1	A	107	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	123	ILE	2.4
1	D	632	TYR	2.4
1	A	103	LYS	2.4
1	D	700	LYS	2.4
1	D	695	SER	2.4
1	C	485	ASP	2.3
1	D	685	ASP	2.3
1	D	724	ASP	2.3
1	D	639	LEU	2.3
1	B	313	GLU	2.3
1	D	643	CYS	2.3
1	B	261	ASP	2.3
1	C	537	ASP	2.3
1	C	442	HIS	2.3
1	B	203	ILE	2.3
1	B	215	VAL	2.3
1	B	250	VAL	2.3
1	C	503	LYS	2.3
1	D	699	LYS	2.3
1	C	534	GLU	2.3
1	A	124	ASP	2.2
1	A	105	PRO	2.2
1	B	235	GLY	2.2
1	A	121	ARG	2.2
1	C	466	ILE	2.2
1	A	47	GLU	2.2
1	D	696	LYS	2.2
1	A	39	LEU	2.1
1	B	265	ASN	2.1
1	C	461	ASP	2.1
1	D	694	SER	2.1
1	C	527	LYS	2.1
1	C	524	ASP	2.1
1	B	280	VAL	2.1
1	B	216	THR	2.1
1	B	245	ILE	2.1
1	B	282	ILE	2.1
1	B	296	LYS	2.1
1	C	523	ILE	2.1
1	A	60	LEU	2.0
1	D	610	ASN	2.0
1	A	83	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	87	VAL	2.0
1	B	334	GLU	2.0
1	C	468	GLU	2.0
1	D	614	ASP	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(Å ²)	Q<0.9
4	TRS	D	807	8/8	0.63	0.16	65,65,66,67	0
2	CA	A	806	1/1	0.81	0.25	29,29,29,29	0
3	SM	B	802	1/1	0.96	0.36	46,46,46,46	0
3	SM	C	804	1/1	0.98	0.37	29,29,29,29	0
2	CA	C	805	1/1	0.98	0.27	13,13,13,13	0
3	SM	B	803	1/1	0.99	0.37	31,31,31,31	0
3	SM	C	801	1/1	1.00	0.28	1,1,1,1	0

6.5 Other polymers [i](#)

There are no such residues in this entry.