Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 08:48 PM EDT

PDB ID	:	1EXZ
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 (i) 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 (1)) were used in the production of this report:

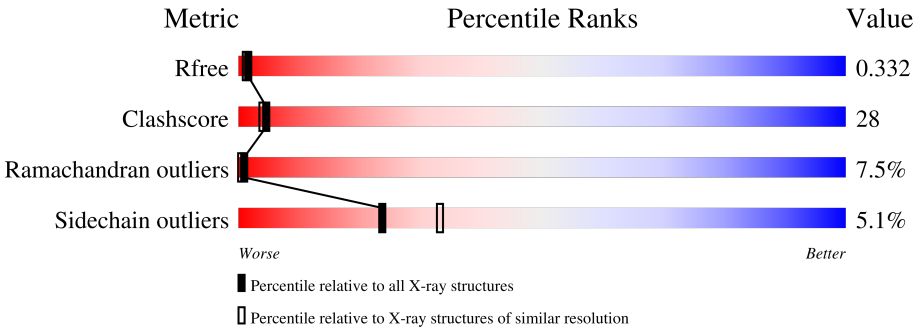
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	141	40% 48% 7% 6%
1	B	141	55% 40% 5% •
1	C	141	57% 29% 6% • 7%
1	D	141	46% 35% 6% • 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			

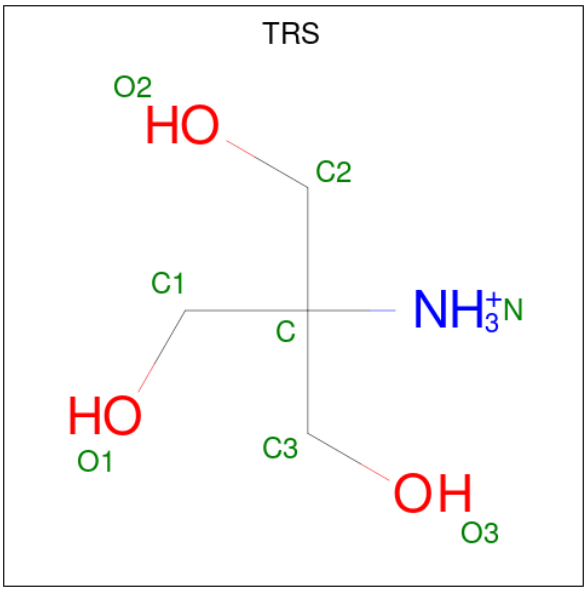
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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 (three-letter code: 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 (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 5 is water.

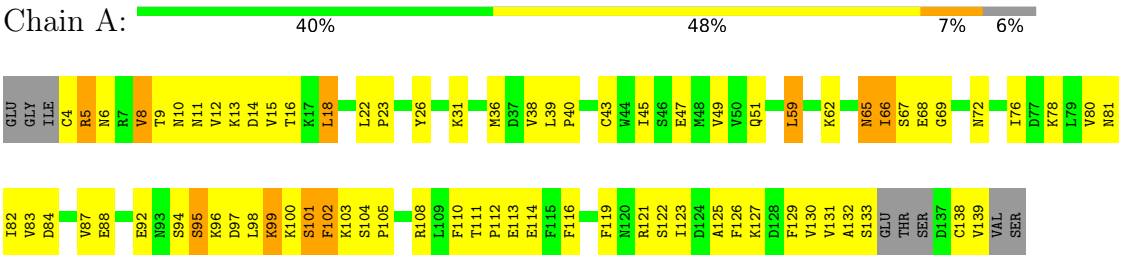
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	35	Total O 35 35	0	0
5	B	32	Total O 32 32	0	0
5	C	37	Total O 37 37	0	0
5	D	28	Total O 28 28	0	0

3 Residue-property plots (i)

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. 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. 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.

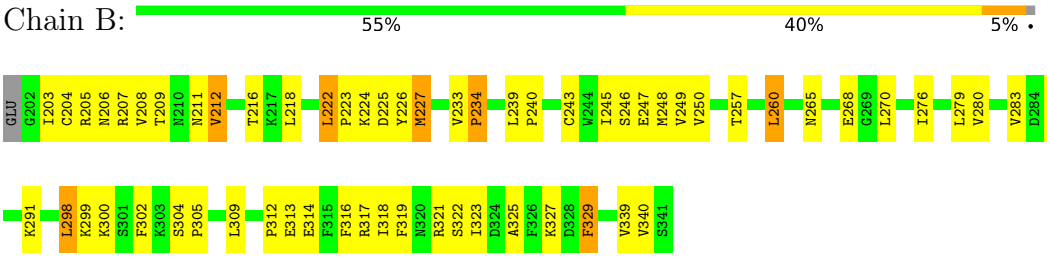
• Molecule 1: STEM CELL FACTOR

Chain A:



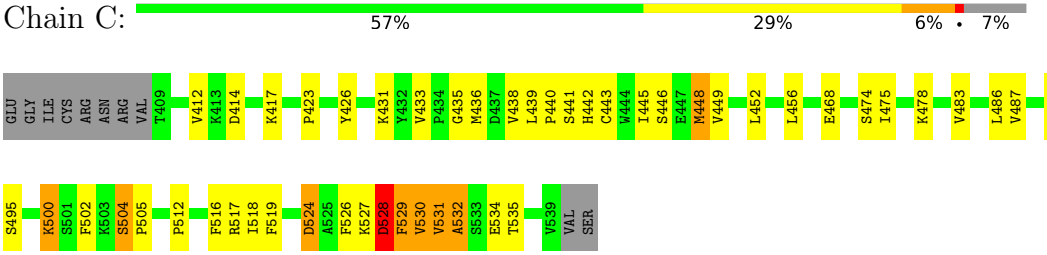
• Molecule 1: STEM CELL FACTOR

Chain B:



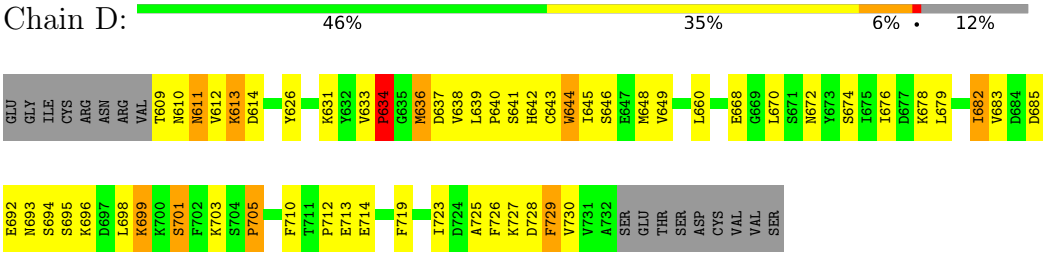
• Molecule 1: STEM CELL FACTOR

Chain C:



• Molecule 1: STEM CELL FACTOR

Chain D:



4 Data and refinement statistics (i)

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 39.35 – 2.29	Depositor EDS
% Data completeness (in resolution range)	10.0 (40.00-2.30) 97.1 (39.35-2.29)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.91 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.294 0.293 , 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)	0.35 , 64.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TRS, CA, SM

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	0.37	0/1067	0.58	0/1444
1	B	0.35	0/1090	0.58	0/1483
1	C	0.39	0/1016	0.62	0/1385
1	D	0.35	0/988	0.56	0/1342
All	All	0.37	0/4161	0.59	0/5654

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	82	1
1	B	1072	0	1033	54	0
1	C	998	0	948	52	0
1	D	971	0	949	50	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	35	0	0	2	0
5	B	32	0	0	1	0
5	C	37	0	0	3	0
5	D	28	0	0	1	0
All	All	4236	0	3983	230	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 28.

All (230) 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: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
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: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	0.70
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:MET:HE2	1:B:248:MET:HA	1.74	0.67
1:B:314:GLU:O	1:B:318:ILE:HD13	1.94	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:A:95:SER:C	1:A:97:ASP:H	1.99	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	0.65
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
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: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: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:436:MET:CE	1:C:518:ILE:HG23	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:686:LEU:HD22	1:D:726:PHE:CD2	2.38	0.57
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:A:12:VAL:HG12	1:A:16:THR:HG1	1.72	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
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: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:C:500:LYS:C	1:C:502:PHE:H	2.11	0.53
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:A:47:GLU:CD	1:A:103:LYS:HA	2.30	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:C:436:MET:HE2	1:C:518:ILE:HG23	1.92	0.51
1:D:726:PHE:C	1:D:728:ASP:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:81:ASN:ND2	5:A:947:HOH:O	2.44	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:4:CYS:O	1:A:5:ARG:C	2.50	0.49
1:A:108:ARG:HG3	1:A:110:PHE:CE1	2.48	0.49
1:C:433:VAL:HG23	1:C:448:MET:HE3	1.94	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: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: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:C:442:HIS:CD2	1:C:534:GLU:HA	2.49	0.47
1:A:95:SER:C	1:A:97:ASP:N	2.64	0.47
1:D:637:ASP:OD1	1:D:638:VAL:HG13	2.13	0.47
1:B:203:ILE:O	1:B:204:CYS:C	2.52	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:260:LEU:HD12	1:B:260:LEU:HA	1.79	0.47
1:D:648:MET:HA	1:D:648:MET:CE	2.45	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:B:248:MET:HE2	1:B:248:MET:CA	2.45	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:B:246:SER:O	1:B:250:VAL:HG23	2.15	0.46
1:C:448:MET:HA	1:C:448:MET:HE3	1.98	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: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:11:ASN:C	1:A:13:LYS:H	2.19	0.45
1:A:111:THR:HG22	1:A:114:GLU:CG	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:MET:HE1	1:C:518:ILE:HG23	1.98	0.45
1:C:529:PHE:HD1	1:C:530:VAL:N	2.02	0.45
1:D:633:VAL:HG23	1:D:648:MET:HE3	1.98	0.45
1:A:97:ASP:O	1:A:99:LYS:N	2.47	0.45
1:A:111:THR:HG22	1:A:114:GLU:CD	2.36	0.45
1:B:211:ASN:ND2	5:B:939:HOH:O	2.49	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:287:VAL:HG12	1:B:287:VAL:O	2.17	0.44
1:A:127:LYS:NZ	1:C:531:VAL:HG13	2.32	0.44
1:D:693:ASN:C	1:D:695:SER:H	2.19	0.44
1:B:318:ILE:HD12	1:B:321:ARG:NH1	2.32	0.44
1:C:524:ASP:C	1:C:526:PHE:H	2.20	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:45:ILE:HD11	1:A:126:PHE:CD1	2.53	0.43
1:B:209:THR:HG22	1:B:211:ASN:CG	2.39	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:26:TYR:O	1:A:112:PRO:HD3	2.18	0.43
1:A:65:ASN:C	1:A:66:ILE:HG12	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:206:ASN:C	1:B:208:VAL:HG23	2.40	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:298:LEU:O	1:B:300:LYS:N	2.49	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:78:LYS:HZ2	1:A:82:ILE:HD11	1.84	0.41
1:D:692:GLU:C	1:D:694:SER:H	2.23	0.41
1:C:436:MET:HE3	5:C:931:HOH:O	2.20	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:A:126:PHE:O	1:A:127:LYS:C	2.59	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:B:329:PHE:C	1:B:329:PHE:CD2	2.94	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:206:ASN:C	1:B:207:ARG:HG2	2.37	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:D:640:PRO:C	1:D:642:HIS:H	2.23	0.40
1:C:527:LYS:HG3	1:C:528:ASP:OD1	2.21	0.40
1:B:223:PRO:C	1:B:225:ASP:H	2.24	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%)	3	2
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

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Mol	Chain	Res	Type
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
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 (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	125/135 (93%)	120 (96%)	5 (4%)	31	44
1	B	121/135 (90%)	112 (93%)	9 (7%)	13	17
1	C	112/135 (83%)	107 (96%)	5 (4%)	27	39
1	D	113/135 (84%)	108 (96%)	5 (4%)	28	39
All	All	471/540 (87%)	447 (95%)	24 (5%)	24	33

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	49	VAL
1	A	59	LEU
1	A	65	ASN
1	A	113	GLU
1	B	212	VAL
1	B	222	LEU
1	B	227	MET
1	B	234	PRO
1	B	239	LEU
1	B	245	ILE
1	B	260	LEU
1	B	270	LEU
1	B	329	PHE
1	C	417	LYS
1	C	448	MET
1	C	524	ASP
1	C	528	ASP
1	C	529	PHE
1	D	613	LYS
1	D	634	PRO
1	D	668	GLU
1	D	670	LEU
1	D	682	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	81	ASN
1	A	120	ASN
1	B	211	ASN
1	B	242	HIS
1	C	442	HIS
1	C	472	ASN
1	C	520	ASN
1	D	642	HIS
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 (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	1.62	1 (14%)	9,9,9	1.29	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	-	-	0/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	807	TRS	C2-C	-3.73	1.41	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	807	TRS	O2-C2-C	2.48	118.85	111.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.