



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:18 PM GMT

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
<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

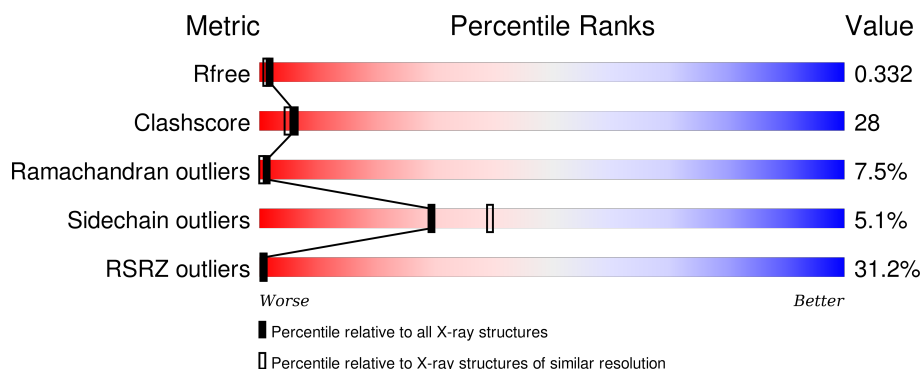
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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	141	
1	B	141	
1	C	141	
1	D	141	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SM	B	802	-	-	-	X
2	SM	B	803	-	-	-	X

2 Entry composition

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			

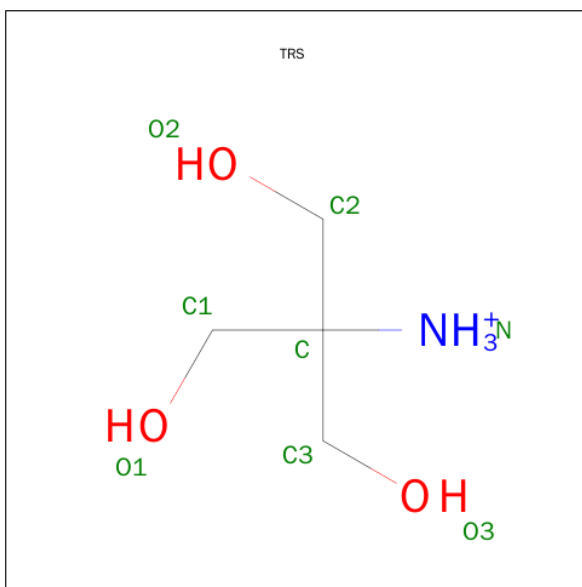
- Molecule 2 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



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

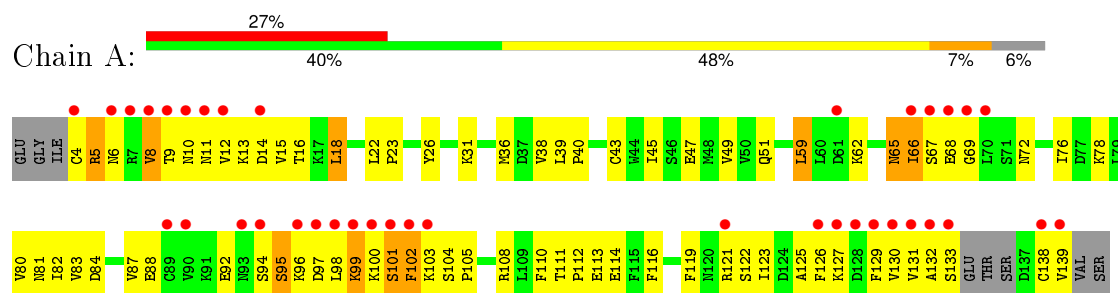
- Molecule 5 is water.

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		

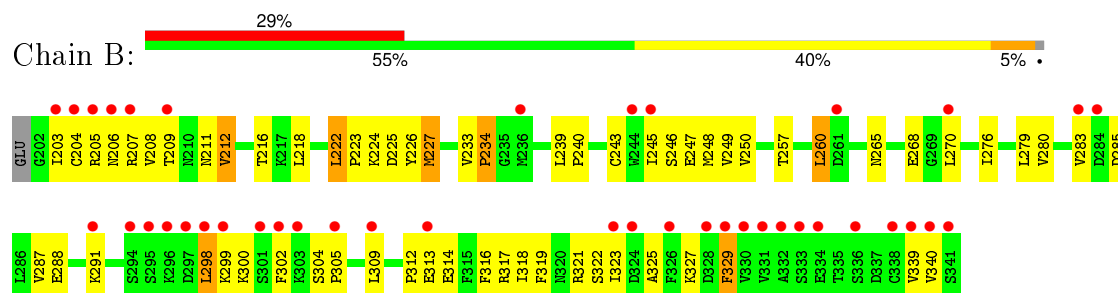
3 Residue-property plots

These plots are drawn for all protein, RNA 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.

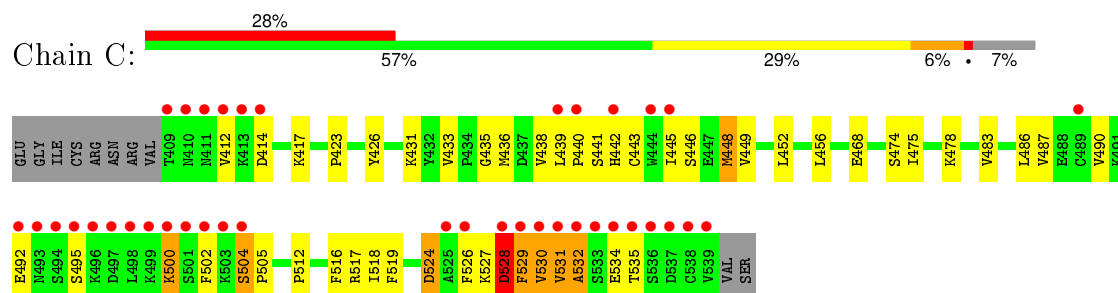
• Molecule 1: STEM CELL FACTOR



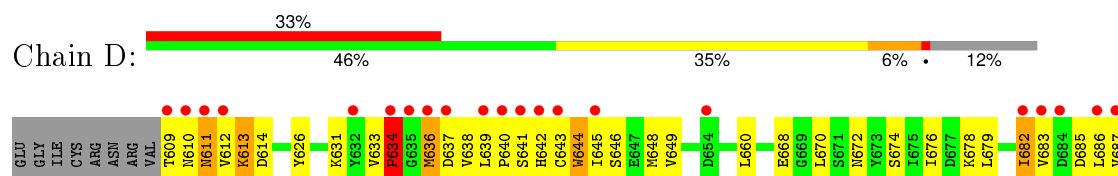
• Molecule 1: STEM CELL FACTOR

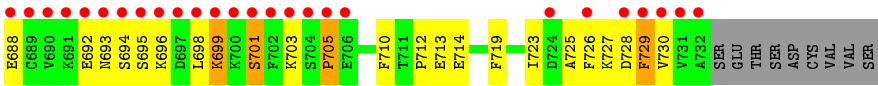


• Molecule 1: STEM CELL FACTOR



• 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 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
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.294 0.292 , 0.332	Depositor DCC
R_{free} test set	1055 reflections (4.91%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 21927 reflections	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.*

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: CA, TRS, 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 [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	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	B	2	0	0	0	1
2	C	2	0	0	0	1
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	D	8	0	11	0	0

Continued on next page...

Continued from previous page...

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:C:532:ALA:HB1	1:C:535:THR:HB	1.69	0.72
1:A:65:ASN:O	1:A:66:ILE:HG23	1.89	0.72
1:A:23:PRO:HG2	1:A:26:TYR:HB2	1.70	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

Continued on next page...

Continued from previous page...

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:C:431:LYS:HB3	1:C:505:PRO:HG2	1.78	0.66
1:A:95:SER:C	1:A:97:ASP:H	1.99	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:O	1:B:208:VAL:HG12	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:B:279:LEU:O	1:B:283:VAL:HG23	2.02	0.59
1:A:78:LYS:NZ	1:A:82:ILE:HD11	2.17	0.59
1:D:633:VAL:HG11	1:D:644:TRP:HB3	1.84	0.59
1:A:12:VAL:HA	1:A:15:VAL:HB	1.85	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:C:504:SER:N	1:C:505:PRO:CD	2.66	0.58
1:A:94:SER:HB2	1:A:99:LYS:HB3	1.84	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

Continued on next page...

Continued from previous page...

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:CE	1:C:448:MET:HA	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:O	1:D:730:VAL:HG12	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:C:441:SER:O	1:C:445:ILE:HG13	2.08	0.53
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: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:94:SER:CB	1:A:99:LYS:HB3	2.39	0.53
1:A:59:LEU:CD1	1:A:76:ILE:HD13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:HH21	1:B:327:LYS:HB2	1.77	0.50
1:A:138:CYS:O	1:A:139:VAL:HB	2.11	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:D:686:LEU:HB3	1:D:726:PHE:CE2	2.47	0.49
1:C:433:VAL:HG23	1:C:448:MET:HE3	1.94	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:C:478:LYS:HE2	5:C:909:HOH:O	2.13	0.48
1:B:240:PRO:HG2	1:B:243:CYS:SG	2.53	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:D:648:MET:CE	1:D:648:MET:HA	2.45	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: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:HG2	1:A:36:MET:O	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:111:THR:HG22	1:A:114:GLU:CG	2.46	0.45
1:A:11:ASN:C	1:A:13:LYS:H	2.19	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:436:MET:HE1	1:C:518:ILE:HG23	1.98	0.45
1:A:111:THR:HG22	1:A:114:GLU:CD	2.36	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:C:486:LEU:HD22	1:C:526:PHE:CZ	2.52	0.45
1:B:218:LEU:HG	1:B:222:LEU:HD22	1.98	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:O	1:B:287:VAL:HG12	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: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:CZ	1:A:123:ILE:HD12	2.53	0.44
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:B:209:THR:HG22	1:B:211:ASN:CG	2.39	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:65:ASN:C	1:A:66:ILE:HG12	2.38	0.43
1:B:204:CYS:SG	1:B:204:CYS:O	2.76	0.43
1:A:26:TYR:O	1:A:112:PRO:HD3	2.18	0.43
1:B:257:THR:O	1:B:260:LEU:HB2	2.19	0.43
1:A:111:THR:CG2	1:A:114:GLU:H	2.20	0.43
1:A:101:SER:O	1:A:102:PHE:CB	2.66	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:D:686:LEU:HD22	1:D:726:PHE:HD2	1.80	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: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

Continued on next page...

Continued from previous page...

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:127:LYS:CE	1:C:531:VAL:HG13	2.50	0.42
1:A:95:SER:O	1:A:96:LYS:HB2	2.19	0.42
1:B:209:THR:O	1:B:211:ASN:ND2	2.52	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:72:ASN:O	1:A:76:ILE:HG13	2.20	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:D:639:LEU:HB3	1:D:640:PRO:HD2	2.01	0.42
1:A:102:PHE:O	1:A:103:LYS:HB3	2.19	0.42
1:C:468:GLU:HB3	5:C:925:HOH:O	2.20	0.42
1:A:62:LYS:O	1:B:224:LYS:HG3	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:126:PHE:O	1:A:127:LYS:C	2.59	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:329:PHE:C	1:B:329:PHE:CD2	2.94	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: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:A:130:VAL:HG23	1:A:131:VAL:HG13	2.03	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	2:B:803:SM:SM[2_645]	2.12	0.08
1:A:88:GLU:OE2	2: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%)	1	0
1	B	138/141 (98%)	113 (82%)	20 (14%)	5 (4%)	4	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%)	1	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

Continued on next page...

Continued from previous page...

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 ⓘ

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%)	38	52
1	B	121/135 (90%)	112 (93%)	9 (7%)	17	21
1	C	112/135 (83%)	107 (96%)	5 (4%)	34	46
1	D	113/135 (84%)	108 (96%)	5 (4%)	35	46
All	All	471/540 (87%)	447 (95%)	24 (5%)	29	39

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

Some 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 carbohydrates 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	2.53	2 (28%)	9,9,9	1.91	4 (44%)

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	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	807	TRS	C2-C	-5.92	1.41	1.53
4	D	807	TRS	C-N	-2.18	1.47	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	807	TRS	C3-C-C1	-2.18	106.05	110.78
4	D	807	TRS	C3-C-C2	2.38	115.93	110.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	807	TRS	O3-C3-C	2.50	116.23	111.18
4	D	807	TRS	O2-C2-C	3.79	118.85	111.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	1.84	38 (28%) 1 1	18, 41, 88, 109	0
1	B	140/141 (99%)	1.90	41 (29%) 1 1	21, 48, 100, 104	0
1	C	131/141 (92%)	2.17	39 (29%) 1 1	18, 37, 92, 119	0
1	D	124/141 (87%)	2.32	47 (37%) 0 0	19, 47, 105, 114	0
All	All	528/564 (93%)	2.05	165 (31%) 1 1	18, 45, 99, 119	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	SER	12.1
1	D	690	VAL	11.8
1	D	700	LYS	11.1
1	B	301	SER	11.0
1	C	529	PHE	10.5
1	C	498	LEU	10.0
1	C	530	VAL	10.0
1	C	502	PHE	9.6
1	B	295	SER	9.6
1	C	495	SER	9.1
1	B	302	PHE	9.0
1	C	532	ALA	8.5
1	A	132	ALA	7.7
1	A	69	GLY	7.7
1	D	701	SER	7.7
1	C	536	SER	7.6
1	B	207	ARG	7.5
1	C	501	SER	7.4
1	D	697	ASP	7.4
1	C	533	SER	7.3
1	A	67	SER	7.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	693	ASN	7.1
1	C	494	SER	7.1
1	C	531	VAL	6.9
1	D	635	GLY	6.8
1	B	298	LEU	6.7
1	D	730	VAL	6.6
1	D	689	CYS	6.6
1	B	297	ASP	6.6
1	B	296	LYS	6.6
1	C	412	VAL	6.4
1	C	500	LYS	6.4
1	D	695	SER	6.3
1	A	8	VAL	6.3
1	A	4	CYS	6.3
1	D	636	MET	6.3
1	D	729	PHE	6.1
1	C	535	THR	6.1
1	B	204	CYS	6.0
1	A	99	LYS	6.0
1	B	330	VAL	5.7
1	D	634	PRO	5.7
1	C	410	ASN	5.6
1	D	694	SER	5.6
1	B	206	ASN	5.4
1	D	728	ASP	5.3
1	D	702	PHE	5.3
1	A	70	LEU	5.2
1	A	68	GLU	5.2
1	A	138	CYS	5.2
1	C	409	THR	5.2
1	D	696	LYS	5.1
1	C	503	LYS	5.1
1	B	294	SER	4.9
1	A	130	VAL	4.9
1	A	7	ARG	4.9
1	B	203	ILE	4.7
1	A	97	ASP	4.7
1	A	131	VAL	4.5
1	B	332	ALA	4.5
1	D	610	ASN	4.4
1	A	102	PHE	4.4
1	C	504	SER	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	100	LYS	4.3
1	D	692	GLU	4.3
1	C	497	ASP	4.3
1	B	291	LYS	4.2
1	D	726	PHE	4.2
1	A	10	ASN	4.2
1	D	731	VAL	4.1
1	B	328	ASP	4.1
1	D	732	ALA	4.1
1	C	539	VAL	4.0
1	A	11	ASN	4.0
1	B	329	PHE	4.0
1	A	98	LEU	4.0
1	A	129	PHE	4.0
1	A	89	CYS	4.0
1	C	534	GLU	3.8
1	D	698	LEU	3.8
1	D	703	LYS	3.8
1	D	643	CYS	3.7
1	D	641	SER	3.7
1	A	6	ASN	3.7
1	D	642	HIS	3.6
1	A	12	VAL	3.6
1	C	528	ASP	3.6
1	A	66	ILE	3.5
1	B	331	VAL	3.5
1	A	9	THR	3.4
1	D	683	VAL	3.4
1	C	537	ASP	3.4
1	A	101	SER	3.4
1	B	305	PRO	3.4
1	B	340	VAL	3.3
1	A	103	LYS	3.3
1	D	691	LYS	3.3
1	C	496	LYS	3.3
1	A	139	VAL	3.3
1	D	705	PRO	3.2
1	D	699	LYS	3.2
1	D	609	THR	3.2
1	D	682	ILE	3.2
1	C	411	ASN	3.2
1	D	687	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	341	SER	3.1
1	D	612	VAL	3.0
1	D	637	ASP	3.0
1	C	492	GLU	3.0
1	C	414	ASP	3.0
1	D	654	ASP	3.0
1	D	688	GLU	3.0
1	C	445	ILE	2.9
1	B	303	LYS	2.9
1	C	413	LYS	2.9
1	A	14	ASP	2.8
1	A	128	ASP	2.8
1	C	526	PHE	2.8
1	B	283	VAL	2.7
1	D	640	PRO	2.7
1	B	339	VAL	2.7
1	B	334	GLU	2.7
1	B	333	SER	2.7
1	D	704	SER	2.7
1	C	493	ASN	2.7
1	D	706	GLU	2.7
1	C	499	LYS	2.7
1	B	236	MET	2.6
1	B	270	LEU	2.6
1	B	324	ASP	2.6
1	A	127	LYS	2.6
1	B	205	ARG	2.6
1	C	525	ALA	2.5
1	B	245	ILE	2.5
1	A	121	ARG	2.5
1	C	538	CYS	2.5
1	A	94	SER	2.4
1	D	686	LEU	2.4
1	B	244	TRP	2.4
1	B	284	ASP	2.4
1	D	639	LEU	2.4
1	B	299	LYS	2.4
1	B	323	ILE	2.4
1	D	684	ASP	2.4
1	A	93	ASN	2.4
1	D	645	ILE	2.4
1	A	126	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	440	PRO	2.4
1	C	439	LEU	2.3
1	D	632	TYR	2.3
1	C	444	TRP	2.3
1	D	724	ASP	2.2
1	B	326	PHE	2.2
1	B	336	SER	2.2
1	D	611	ASN	2.2
1	C	489	CYS	2.2
1	A	90	VAL	2.1
1	B	261	ASP	2.1
1	B	309	LEU	2.1
1	B	209	THR	2.1
1	A	96	LYS	2.1
1	B	338	CYS	2.0
1	A	61	ASP	2.0
1	B	313	GLU	2.0
1	C	442	HIS	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(Å ²)	Q<0.9
2	SM	B	803	1/1	0.98	0.36	3.19	31,31,31,31	0
3	CA	C	805	1/1	0.95	0.27	1.72	13,13,13,13	0
2	SM	B	802	1/1	0.98	0.40	0.72	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SM	C	804	1/1	0.98	0.38	-0.82	29,29,29,29	0
3	CA	A	806	1/1	0.87	0.33	-	29,29,29,29	0
4	TRS	D	807	8/8	0.57	0.34	-	65,65,66,67	0
2	SM	C	801	1/1	0.99	0.21	-	1,1,1,1	0

6.5 Other polymers [i](#)

There are no such residues in this entry.