



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:11 AM UTC

PDB ID : 3DBN / pdb_00003dbn
Title : Crystal structure of the Streptococcus suis serotype2 D-mannonate dehydratase in complex with its substrate
Authors : Peng, H.; Zhang, Q.; Gao, F.; Gao, G.F.
Deposited on : 2008-06-02
Resolution : 2.90 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

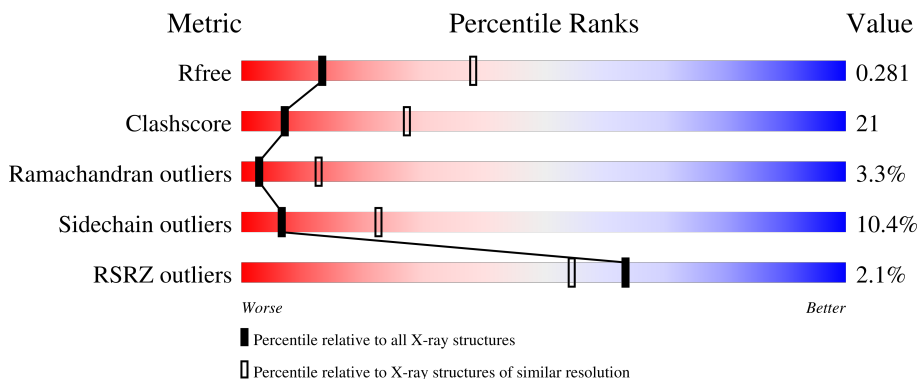
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	386	% 49% 34% 7% 10%
1	B	386	3% 49% 34% 6% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5484 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 Mannonate dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2737	1745	465	513	14			
1	B	349	Total	C	N	O	S	0	0	0
			2732	1742	465	512	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP A4VVI4
A	2	GLY	-	expression tag	UNP A4VVI4
A	3	SER	-	expression tag	UNP A4VVI4
A	4	SER	-	expression tag	UNP A4VVI4
A	5	HIS	-	expression tag	UNP A4VVI4
A	6	HIS	-	expression tag	UNP A4VVI4
A	7	HIS	-	expression tag	UNP A4VVI4
A	8	HIS	-	expression tag	UNP A4VVI4
A	9	HIS	-	expression tag	UNP A4VVI4
A	10	HIS	-	expression tag	UNP A4VVI4
A	11	SER	-	expression tag	UNP A4VVI4
A	12	SER	-	expression tag	UNP A4VVI4
A	13	GLY	-	expression tag	UNP A4VVI4
A	14	LEU	-	expression tag	UNP A4VVI4
A	15	VAL	-	expression tag	UNP A4VVI4
A	16	PRO	-	expression tag	UNP A4VVI4
A	17	ARG	-	expression tag	UNP A4VVI4
A	18	GLY	-	expression tag	UNP A4VVI4
A	19	SER	-	expression tag	UNP A4VVI4
A	20	HIS	-	expression tag	UNP A4VVI4
B	1	MET	-	expression tag	UNP A4VVI4
B	2	GLY	-	expression tag	UNP A4VVI4
B	3	SER	-	expression tag	UNP A4VVI4
B	4	SER	-	expression tag	UNP A4VVI4
B	5	HIS	-	expression tag	UNP A4VVI4

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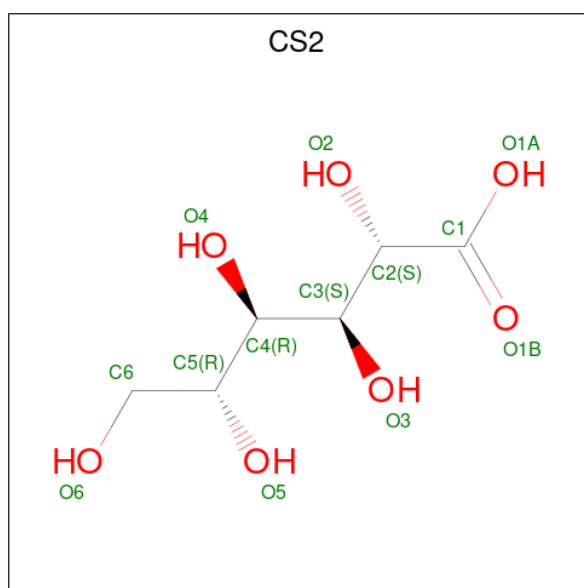
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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	expression tag	UNP A4VVI4
B	7	HIS	-	expression tag	UNP A4VVI4
B	8	HIS	-	expression tag	UNP A4VVI4
B	9	HIS	-	expression tag	UNP A4VVI4
B	10	HIS	-	expression tag	UNP A4VVI4
B	11	SER	-	expression tag	UNP A4VVI4
B	12	SER	-	expression tag	UNP A4VVI4
B	13	GLY	-	expression tag	UNP A4VVI4
B	14	LEU	-	expression tag	UNP A4VVI4
B	15	VAL	-	expression tag	UNP A4VVI4
B	16	PRO	-	expression tag	UNP A4VVI4
B	17	ARG	-	expression tag	UNP A4VVI4
B	18	GLY	-	expression tag	UNP A4VVI4
B	19	SER	-	expression tag	UNP A4VVI4
B	20	HIS	-	expression tag	UNP A4VVI4

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0

- Molecule 3 is D-MANNONIC ACID (CCD ID: CS2) (formula: C₆H₁₂O₇).

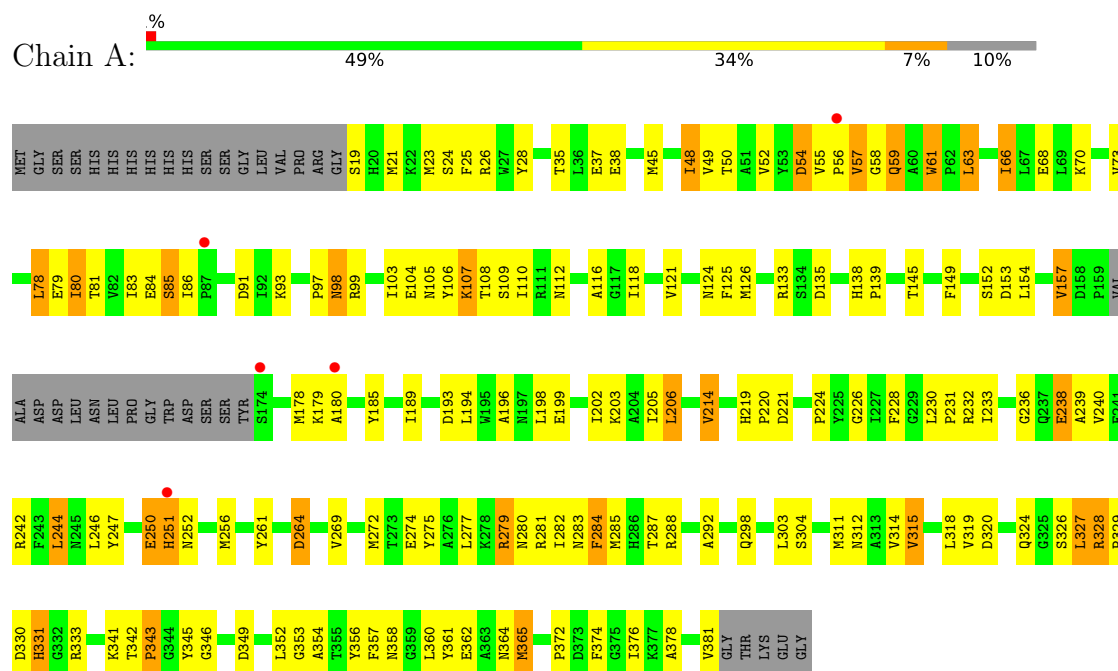


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

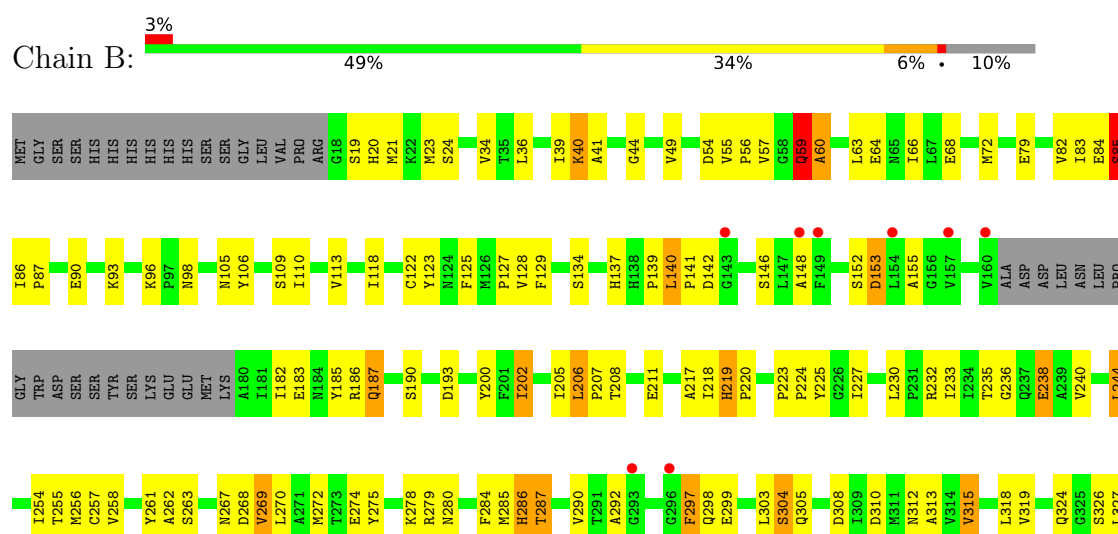
3 Residue-property plots

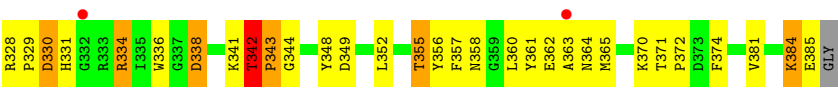
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Mannonate dehydratase



• Molecule 1: Mannonate dehydratase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.52Å 105.52Å 160.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.8 (50.00-2.90) 95.8 (50.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.03 (at 2.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.231 , 0.280 0.230 , 0.281	Depositor DCC
R_{free} test set	981 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	5484	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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: MN, CS2

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	0.81	0/2804	1.12	11/3807 (0.3%)
1	B	0.82	0/2799	1.16	20/3801 (0.5%)
All	All	0.82	0/5603	1.14	31/7608 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	342	THR	CA-C-N	9.85	132.15	119.84
1	B	342	THR	C-N-CA	9.85	132.15	119.84
1	A	304	SER	N-CA-C	7.32	119.26	111.28
1	B	292	ALA	N-CA-C	6.95	117.76	108.38
1	A	61	TRP	CA-C-N	-6.28	113.48	119.76
1	A	61	TRP	C-N-CA	-6.28	113.48	119.76
1	A	157	VAL	N-CA-C	6.28	117.07	107.77
1	B	219	HIS	CA-C-N	6.12	127.49	119.84
1	B	219	HIS	C-N-CA	6.12	127.49	119.84
1	A	55	VAL	CA-C-N	6.11	127.47	119.84
1	A	55	VAL	C-N-CA	6.11	127.47	119.84
1	B	297	PHE	N-CA-C	5.96	118.91	109.50
1	A	264	ASP	CA-C-N	5.91	126.32	119.47
1	A	264	ASP	C-N-CA	5.91	126.32	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	VAL	CA-C-N	5.82	125.84	119.90
1	B	55	VAL	C-N-CA	5.82	125.84	119.90
1	A	292	ALA	N-CA-C	5.69	115.53	108.19
1	B	269	VAL	N-CA-C	5.64	116.42	110.72
1	B	41	ALA	CA-C-N	-5.62	118.78	122.60
1	B	41	ALA	C-N-CA	-5.62	118.78	122.60
1	B	200	TYR	N-CA-C	-5.51	104.96	110.97
1	A	236	GLY	N-CA-C	5.41	118.43	110.80
1	B	59	GLN	N-CA-C	5.40	120.14	113.50
1	A	55	VAL	N-CA-C	5.32	113.79	107.73
1	B	286	HIS	N-CA-C	-5.28	101.67	110.17
1	B	206	LEU	CA-C-N	-5.22	113.53	119.28
1	B	206	LEU	C-N-CA	-5.22	113.53	119.28
1	B	96	LYS	CA-C-N	5.08	126.20	119.84
1	B	96	LYS	C-N-CA	5.08	126.20	119.84
1	B	140	LEU	CA-C-N	5.05	126.16	119.84
1	B	140	LEU	C-N-CA	5.05	126.16	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	85	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2737	0	2676	126	0
1	B	2732	0	2678	109	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	10	2	0
All	All	5484	0	5364	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 21.

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:B:182:ILE:HG22	1:B:186:ARG:HD2	1.31	1.06
1:B:287:THR:HG23	1:B:287:THR:O	1.57	1.01
1:A:21:MET:HE3	1:A:23:MET:HE1	1.46	0.95
1:A:226:GLY:HA2	1:A:232:ARG:HD3	1.48	0.94
1:A:57:VAL:HG13	1:A:58:GLY:H	1.30	0.92
1:A:250:GLU:HG2	1:A:280:ASN:HD22	1.31	0.92
1:A:21:MET:HE3	1:A:23:MET:CE	1.99	0.91
1:A:194:LEU:HD23	1:A:233:ILE:HG12	1.51	0.91
1:B:56:PRO:O	1:B:59:GLN:HB2	1.71	0.90
1:B:21:MET:HE3	1:B:361:TYR:CD2	2.08	0.88
1:B:287:THR:O	1:B:287:THR:CG2	2.25	0.84
1:B:57:VAL:HG13	1:B:87:PRO:HB2	1.61	0.81
1:A:21:MET:CE	1:A:23:MET:HE1	2.10	0.80
1:B:36:LEU:HA	1:B:39:ILE:HD12	1.64	0.78
1:B:236:GLY:HA3	1:B:267:ASN:HD21	1.52	0.75
1:A:330:ASP:O	1:A:331:HIS:O	2.06	0.73
1:A:57:VAL:HG13	1:A:58:GLY:N	2.04	0.73
1:A:19:SER:N	1:A:324:GLN:HE21	1.87	0.72
1:A:104:GLU:HA	1:A:107:LYS:HG3	1.73	0.71
1:A:250:GLU:HG3	1:A:281:ARG:NH1	2.06	0.70
1:B:182:ILE:HG22	1:B:186:ARG:CD	2.18	0.70
1:A:49:VAL:HG13	1:A:84:GLU:HB2	1.75	0.69
1:B:140:LEU:HD11	1:B:146:SER:HB3	1.73	0.69
1:A:121:VAL:HG23	1:A:214:VAL:CG1	2.23	0.68
1:A:121:VAL:HG23	1:A:214:VAL:HG13	1.76	0.68
1:B:236:GLY:O	1:B:240:VAL:HG23	1.95	0.67
1:B:287:THR:HG21	1:B:327:LEU:HD21	1.77	0.67
1:A:312:ASN:HD21	1:A:364:ASN:HD21	1.42	0.66
1:A:220:PRO:HB3	1:A:261:TYR:CZ	2.30	0.66
1:B:49:VAL:HG22	1:B:82:VAL:HB	1.77	0.66
1:A:283:ASN:O	1:A:284:PHE:HB2	1.96	0.66
1:B:236:GLY:HA3	1:B:267:ASN:ND2	2.10	0.65
1:A:48:ILE:HG21	1:A:73:VAL:HG11	1.79	0.65
1:A:57:VAL:CG1	1:A:58:GLY:H	2.07	0.65
1:B:287:THR:HG23	1:B:357:PHE:CZ	2.33	0.64
1:B:286:HIS:CE1	1:B:328:ARG:HH11	2.16	0.64
1:A:26:ARG:HA	1:A:49:VAL:HB	1.79	0.64
1:A:312:ASN:ND2	1:A:364:ASN:HD21	1.95	0.64
1:A:250:GLU:HG3	1:A:281:ARG:HH12	1.63	0.63
1:A:352:LEU:HD22	1:B:355:THR:CG2	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASP:HB3	1:A:98:ASN:HD21	1.62	0.63
1:A:199:GLU:O	1:A:203:LYS:HG2	1.99	0.63
1:A:288:ARG:HD3	1:A:330:ASP:HB3	1.80	0.63
1:B:23:MET:HE3	1:B:358:ASN:OD1	1.99	0.62
1:B:105:ASN:O	1:B:109:SER:OG	2.16	0.62
1:A:66:ILE:HD11	1:A:116:ALA:CB	2.29	0.61
1:A:73:VAL:HG13	1:A:78:LEU:HB2	1.81	0.61
1:A:84:GLU:O	1:A:85:SER:HB2	2.01	0.61
1:B:205:ILE:O	1:B:208:THR:HB	1.99	0.61
1:B:182:ILE:CG2	1:B:186:ARG:HD2	2.19	0.60
1:B:90:GLU:OE2	1:B:128:VAL:N	2.29	0.60
1:A:206:LEU:HB3	1:A:247:TYR:CZ	2.36	0.60
1:B:330:ASP:O	1:B:331:HIS:HB2	2.01	0.60
1:A:21:MET:HE3	1:A:23:MET:HE2	1.82	0.59
1:B:183:GLU:HA	1:B:186:ARG:HB2	1.85	0.59
1:A:193:ASP:O	1:A:196:ALA:HB3	2.01	0.59
1:B:106:TYR:O	1:B:110:ILE:HG13	2.02	0.59
1:B:235:THR:O	1:B:267:ASN:ND2	2.36	0.59
1:A:125:PHE:CG	1:A:198:LEU:HD13	2.38	0.58
1:A:311:MET:O	1:A:315:VAL:HG12	2.04	0.58
1:A:358:ASN:HD22	1:A:374:PHE:HE1	1.53	0.57
1:A:25:PHE:HB2	1:A:45:MET:SD	2.45	0.57
1:A:314:VAL:O	1:A:318:LEU:HG	2.04	0.57
1:B:331:HIS:HA	1:B:344:GLY:O	2.05	0.57
1:B:40:LYS:HD3	1:B:40:LYS:O	2.04	0.56
1:A:49:VAL:CG1	1:A:84:GLU:HB2	2.35	0.56
1:A:352:LEU:HD22	1:B:355:THR:HG21	1.85	0.56
1:B:85:SER:HA	1:B:122:CYS:O	2.06	0.56
1:A:135:ASP:OD2	1:A:138:HIS:ND1	2.33	0.56
1:B:123:TYR:CE1	1:B:218:ILE:HD12	2.40	0.56
1:B:83:ILE:HG12	1:B:118:ILE:HG21	1.88	0.56
1:B:312:ASN:ND2	1:B:364:ASN:HD21	2.04	0.55
1:A:35:THR:HB	1:A:38:GLU:HG3	1.88	0.55
1:B:310:ASP:OD1	1:B:313:ALA:HB2	2.05	0.55
1:A:372:PRO:HG2	1:B:305:GLN:HE22	1.72	0.55
1:B:284:PHE:CE1	1:B:286:HIS:HE1	2.25	0.55
1:A:104:GLU:CD	1:A:107:LYS:HZ3	2.14	0.55
1:A:54:ASP:OD1	1:A:54:ASP:N	2.39	0.55
1:A:80:ILE:HG21	1:A:118:ILE:HD13	1.88	0.55
1:A:312:ASN:HD22	1:A:360:LEU:HD22	1.72	0.54
1:B:356:TYR:CZ	1:B:360:LEU:HD11	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LEU:HD11	1:A:252:ASN:HB2	1.89	0.54
1:A:231:PRO:C	1:A:232:ARG:HD2	2.33	0.54
1:B:20:HIS:H	1:B:324:GLN:HG2	1.73	0.53
1:A:99:ARG:O	1:A:103:ILE:HG13	2.08	0.53
1:B:153:ASP:OD1	1:B:153:ASP:N	2.41	0.53
1:B:319:VAL:HG21	1:B:364:ASN:HB3	1.90	0.53
1:A:116:ALA:O	1:A:118:ILE:HG13	2.09	0.53
1:B:262:ALA:HB2	1:B:269:VAL:CG1	2.39	0.52
1:A:288:ARG:HD2	1:A:331:HIS:HB2	1.90	0.52
1:A:288:ARG:HH11	1:A:288:ARG:HG2	1.73	0.52
1:B:56:PRO:HB2	1:B:59:GLN:HG3	1.92	0.52
1:B:187:GLN:OE1	1:B:187:GLN:HA	2.10	0.52
1:A:126:MET:HE2	1:A:221:ASP:HA	1.91	0.52
1:B:217:ALA:HB1	1:B:255:THR:OG1	2.10	0.52
1:A:35:THR:HG22	1:A:37:GLU:H	1.75	0.52
1:B:244:LEU:HB3	1:B:279:ARG:NH1	2.25	0.52
1:A:319:VAL:HG13	1:A:365:MET:CE	2.39	0.51
1:B:275:TYR:OH	1:B:279:ARG:NH2	2.43	0.51
1:A:91:ASP:CB	1:A:98:ASN:HD21	2.23	0.51
1:A:331:HIS:CD2	1:A:331:HIS:H	2.28	0.51
1:A:103:ILE:O	1:A:107:LYS:HG2	2.11	0.51
1:A:224:PRO:HG2	1:A:264:ASP:HB2	1.93	0.51
1:B:285:MET:O	1:B:327:LEU:HA	2.10	0.51
1:B:127:PRO:HB3	1:B:185:TYR:CZ	2.45	0.51
1:A:97:PRO:C	1:A:99:ARG:H	2.19	0.51
1:A:376:ILE:HG21	1:B:305:GLN:O	2.12	0.50
1:A:73:VAL:CG1	1:A:78:LEU:HB2	2.42	0.50
1:B:137:HIS:O	1:B:139:PRO:HD3	2.12	0.50
1:A:149:PHE:HE1	1:A:154:LEU:HD22	1.76	0.50
1:B:153:ASP:C	1:B:155:ALA:H	2.19	0.50
1:A:277:LEU:CD2	1:A:282:ILE:HD12	2.42	0.49
1:B:148:ALA:HB2	1:B:298:GLN:HG3	1.93	0.49
1:B:299:GLU:OE2	1:B:331:HIS:HD2	1.96	0.49
1:A:303:LEU:HA	1:A:356:TYR:CZ	2.48	0.49
1:A:342:THR:O	1:A:343:PRO:C	2.55	0.49
1:B:206:LEU:O	1:B:207:PRO:C	2.53	0.49
1:B:262:ALA:HB2	1:B:269:VAL:HG11	1.95	0.48
1:A:319:VAL:HG13	1:A:365:MET:HE3	1.94	0.48
1:B:238:GLU:CD	1:B:238:GLU:H	2.21	0.48
1:A:59:GLN:C	1:A:105:ASN:HB3	2.39	0.48
1:A:261:TYR:HB3	1:A:272:MET:HE1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:GLU:OE2	1:B:304:SER:OG	2.18	0.48
1:A:63:LEU:H	1:A:112:ASN:HD22	1.62	0.48
1:B:256:MET:HB3	1:B:285:MET:SD	2.54	0.48
1:B:129:PHE:HB2	1:B:232:ARG:NH1	2.29	0.48
1:A:345:TYR:HE1	3:A:388:CS2:H61	1.78	0.47
1:A:287:THR:HG23	1:A:357:PHE:CZ	2.49	0.47
1:A:372:PRO:HG2	1:B:305:GLN:NE2	2.29	0.47
1:A:61:TRP:CZ3	1:A:83:ILE:HG21	2.49	0.47
1:B:24:SER:O	1:B:329:PRO:HD2	2.14	0.47
1:B:275:TYR:HD1	1:B:278:LYS:NZ	2.13	0.46
1:B:223:PRO:O	1:B:225:TYR:N	2.40	0.46
1:B:275:TYR:O	1:B:278:LYS:HB2	2.15	0.46
1:A:93:LYS:HE2	1:A:125:PHE:HA	1.97	0.46
1:B:275:TYR:HD1	1:B:278:LYS:HZ2	1.61	0.46
1:B:342:THR:HA	1:B:343:PRO:HD2	1.66	0.46
1:B:49:VAL:CG1	1:B:84:GLU:HB2	2.45	0.46
1:B:82:VAL:HG11	1:B:284:PHE:CE1	2.51	0.46
1:A:108:THR:OG1	1:A:109:SER:N	2.49	0.46
1:B:23:MET:SD	1:B:327:LEU:HD22	2.56	0.46
1:B:312:ASN:HD21	1:B:364:ASN:HD21	1.62	0.46
1:A:79:GLU:O	1:A:79:GLU:HG3	2.16	0.46
1:A:219:HIS:CE1	3:A:388:CS2:O1B	2.68	0.46
1:B:263:SER:HB2	1:B:297:PHE:CD1	2.50	0.46
1:B:365:MET:O	1:B:370:LYS:HB2	2.15	0.46
1:A:63:LEU:N	1:A:112:ASN:HD22	2.13	0.46
1:B:182:ILE:HG23	1:B:230:LEU:HD21	1.98	0.46
1:A:61:TRP:HB2	1:A:109:SER:HA	1.98	0.45
1:A:329:PRO:HG3	1:A:354:ALA:HA	1.98	0.45
1:B:223:PRO:C	1:B:225:TYR:H	2.24	0.45
1:B:59:GLN:O	1:B:60:ALA:HB3	2.17	0.45
1:B:267:ASN:HB3	1:B:272:MET:CE	2.46	0.45
1:A:199:GLU:HG3	1:A:246:LEU:HD22	1.97	0.45
1:A:319:VAL:HG22	1:A:365:MET:HE3	1.97	0.45
1:B:142:ASP:OD1	1:B:142:ASP:C	2.60	0.45
1:A:303:LEU:HD11	1:B:374:PHE:CE2	2.52	0.45
1:A:283:ASN:O	1:A:284:PHE:CB	2.65	0.45
1:A:133:ARG:HG2	1:A:133:ARG:HH11	1.83	0.44
1:B:207:PRO:O	1:B:211:GLU:HG3	2.17	0.44
1:B:365:MET:HG3	1:B:372:PRO:HB3	1.99	0.44
1:A:124:ASN:OD1	1:A:124:ASN:C	2.60	0.44
1:A:269:VAL:HA	1:A:272:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:GLU:O	1:A:275:TYR:C	2.60	0.44
1:B:315:VAL:O	1:B:318:LEU:N	2.51	0.44
1:A:287:THR:HG23	1:A:287:THR:O	2.17	0.44
1:A:333:ARG:HD3	1:A:349:ASP:OD2	2.18	0.44
1:B:349:ASP:HA	1:B:352:LEU:HG	1.98	0.44
1:A:24:SER:OG	1:A:326:SER:HB2	2.18	0.44
1:A:284:PHE:HD2	1:A:326:SER:O	2.00	0.44
1:B:190:SER:H	1:B:193:ASP:HB2	1.82	0.44
1:A:48:ILE:HG22	1:A:80:ILE:N	2.32	0.44
1:A:178:MET:C	1:A:180:ALA:N	2.76	0.44
1:A:353:GLY:O	1:A:354:ALA:C	2.60	0.44
1:B:190:SER:N	1:B:193:ASP:HB2	2.33	0.44
1:B:284:PHE:CE1	1:B:286:HIS:CE1	3.06	0.43
1:A:139:PRO:HA	1:A:145:THR:HG22	2.01	0.43
1:B:256:MET:HG3	1:B:258:VAL:HG13	2.00	0.43
1:A:104:GLU:O	1:A:107:LYS:HB2	2.18	0.43
1:A:50:THR:O	1:A:83:ILE:HA	2.17	0.43
1:B:63:LEU:HA	1:B:66:ILE:HD12	2.00	0.43
1:A:106:TYR:O	1:A:110:ILE:HG13	2.19	0.43
1:A:251:HIS:ND1	1:A:251:HIS:N	2.66	0.43
1:A:328:ARG:NH2	1:A:345:TYR:HE2	2.16	0.43
1:A:356:TYR:OH	1:B:362:GLU:OE1	2.24	0.43
1:B:109:SER:O	1:B:113:VAL:HG23	2.18	0.43
1:B:334:ARG:HG2	1:B:338:ASP:HB3	2.01	0.43
1:B:356:TYR:O	1:B:360:LEU:HG	2.19	0.43
1:B:261:TYR:HB3	1:B:272:MET:HE1	2.00	0.43
1:A:330:ASP:O	1:A:331:HIS:C	2.62	0.43
1:A:362:GLU:HG3	1:A:372:PRO:HG3	2.01	0.43
1:B:336:TRP:CH2	1:B:352:LEU:HD21	2.53	0.42
1:A:110:ILE:HD12	1:A:205:ILE:HB	2.01	0.42
1:A:315:VAL:HG11	1:A:360:LEU:HB3	2.01	0.42
1:A:327:LEU:HD23	1:A:327:LEU:C	2.44	0.42
1:B:137:HIS:HD2	1:B:334:ARG:HH21	1.68	0.42
1:A:108:THR:O	1:A:109:SER:C	2.62	0.42
1:A:179:LYS:O	1:A:179:LYS:HG2	2.19	0.42
1:A:378:ALA:O	1:B:141:PRO:HG3	2.19	0.42
1:B:44:GLY:HA2	1:B:374:PHE:HB3	2.01	0.42
1:B:54:ASP:OD1	1:B:54:ASP:N	2.49	0.42
1:A:228:PHE:C	1:A:230:LEU:H	2.27	0.42
1:B:93:LYS:HE2	1:B:125:PHE:HA	2.02	0.42
1:A:238:GLU:H	1:A:238:GLU:HG3	1.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:SER:OG	1:A:81:THR:HG21	2.20	0.42
1:A:256:MET:HB3	1:A:285:MET:SD	2.60	0.42
1:B:219:HIS:HE1	1:B:286:HIS:HD2	1.68	0.41
1:A:185:TYR:HA	1:A:189:ILE:HB	2.01	0.41
1:A:121:VAL:CG2	1:A:214:VAL:HG11	2.50	0.41
1:A:279:ARG:HE	1:A:279:ARG:HB3	1.40	0.41
1:A:239:ALA:O	1:A:240:VAL:C	2.63	0.41
1:A:328:ARG:NH2	1:A:330:ASP:OD1	2.54	0.41
1:B:336:TRP:HH2	1:B:352:LEU:HD21	1.85	0.41
1:B:64:GLU:OE1	1:B:64:GLU:N	2.53	0.41
1:B:68:GLU:O	1:B:72:MET:HG3	2.19	0.41
1:B:310:ASP:OD1	1:B:313:ALA:CB	2.69	0.41
1:B:257:CYS:HA	1:B:286:HIS:HB2	2.03	0.41
1:A:121:VAL:HG23	1:A:214:VAL:HG11	2.01	0.40
1:B:202:ILE:HA	1:B:205:ILE:HG12	2.02	0.40
1:B:284:PHE:HD2	1:B:326:SER:O	2.04	0.40
1:A:23:MET:HG3	1:A:45:MET:HE1	2.01	0.40
1:A:52:VAL:CG1	1:A:54:ASP:OD1	2.69	0.40
1:A:244:LEU:HG	1:A:281:ARG:HG3	2.02	0.40
1:B:40:LYS:HD3	1:B:40:LYS:C	2.46	0.40
1:B:270:LEU:HD21	1:B:313:ALA:HB3	2.02	0.40
1:B:384:LYS:HG3	1:B:385:GLU:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	345/386 (89%)	290 (84%)	43 (12%)	12 (4%)	3	12
1	B	345/386 (89%)	301 (87%)	33 (10%)	11 (3%)	3	13
All	All	690/772 (89%)	591 (86%)	76 (11%)	23 (3%)	3	13

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	A	284	PHE
1	A	331	HIS
1	A	343	PRO
1	B	343	PRO
1	A	28	TYR
1	A	85	SER
1	A	346	GLY
1	B	330	ASP
1	B	60	ALA
1	B	220	PRO
1	B	384	LYS
1	A	56	PRO
1	A	98	ASN
1	B	224	PRO
1	B	304	SER
1	B	348	TYR
1	A	361	TYR
1	B	338	ASP
1	B	363	ALA
1	A	68	GLU
1	B	85	SER
1	A	214	VAL

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	288/321 (90%)	259 (90%)	29 (10%)	7	24
1	B	288/321 (90%)	257 (89%)	31 (11%)	6	21
All	All	576/642 (90%)	516 (90%)	60 (10%)	7	23

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ILE
1	A	54	ASP
1	A	59	GLN
1	A	63	LEU
1	A	66	ILE
1	A	70	LYS
1	A	78	LEU
1	A	80	ILE
1	A	86	ILE
1	A	107	LYS
1	A	152	SER
1	A	153	ASP
1	A	157	VAL
1	A	202	ILE
1	A	206	LEU
1	A	238	GLU
1	A	242	ARG
1	A	244	LEU
1	A	250	GLU
1	A	251	HIS
1	A	279	ARG
1	A	298	GLN
1	A	315	VAL
1	A	320	ASP
1	A	327	LEU
1	A	328	ARG
1	A	341	LYS
1	A	365	MET
1	A	381	VAL
1	B	19	SER
1	B	34	VAL
1	B	40	LYS
1	B	59	GLN
1	B	79	GLU
1	B	86	ILE
1	B	98	ASN
1	B	134	SER
1	B	152	SER
1	B	153	ASP
1	B	187	GLN
1	B	202	ILE
1	B	227	ILE
1	B	233	ILE

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Mol	Chain	Res	Type
1	B	238	GLU
1	B	244	LEU
1	B	254	ILE
1	B	268	ASP
1	B	274	GLU
1	B	280	ASN
1	B	287	THR
1	B	290	VAL
1	B	303	LEU
1	B	308	ASP
1	B	315	VAL
1	B	334	ARG
1	B	341	LYS
1	B	342	THR
1	B	355	THR
1	B	371	THR
1	B	381	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	105	ASN
1	A	112	ASN
1	A	197	ASN
1	A	252	ASN
1	A	280	ASN
1	A	298	GLN
1	A	305	GLN
1	A	312	ASN
1	A	364	ASN
1	B	59	GLN
1	B	98	ASN
1	B	105	ASN
1	B	137	HIS
1	B	184	ASN
1	B	188	ASN
1	B	219	HIS
1	B	267	ASN
1	B	283	ASN
1	B	286	HIS
1	B	305	GLN

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Mol	Chain	Res	Type
1	B	312	ASN
1	B	324	GLN
1	B	331	HIS
1	B	364	ASN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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	$\# Z > 2$
3	CS2	A	388	2	12,12,12	1.11	1 (8%)	15,16,16	1.23	3 (20%)

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
3	CS2	A	388	2	-	11/18/18/18	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	388	CS2	C2-C1	2.26	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	388	CS2	O3-C3-C2	-2.26	105.23	109.29
3	A	388	CS2	O1A-C1-C2	2.22	119.48	113.31
3	A	388	CS2	O1B-C1-C2	-2.08	116.07	121.62

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	388	CS2	C1-C2-C3-C4
3	A	388	CS2	C4-C5-C6-O6
3	A	388	CS2	O2-C2-C3-C4
3	A	388	CS2	O1B-C1-C2-C3
3	A	388	CS2	O5-C5-C6-O6
3	A	388	CS2	O1A-C1-C2-C3
3	A	388	CS2	O2-C2-C3-O3
3	A	388	CS2	C1-C2-C3-O3
3	A	388	CS2	C3-C4-C5-C6
3	A	388	CS2	O1B-C1-C2-O2
3	A	388	CS2	O1A-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	388	CS2	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	349/386 (90%)	-0.03	5 (1%) 73 65	3, 22, 42, 49	0
1	B	349/386 (90%)	-0.02	10 (2%) 53 45	2, 20, 42, 63	0
All	All	698/772 (90%)	-0.02	15 (2%) 63 54	2, 21, 42, 63	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	ALA	4.6
1	B	143	GLY	3.0
1	B	160	VAL	2.8
1	A	174	SER	2.8
1	A	87	PRO	2.6
1	B	293	GLY	2.5
1	B	157	VAL	2.5
1	B	363	ALA	2.5
1	A	180	ALA	2.4
1	A	251	HIS	2.4
1	A	56	PRO	2.3
1	B	154	LEU	2.3
1	B	296	GLY	2.2
1	B	332	GLY	2.1
1	B	149	PHE	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

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
3	CS2	A	388	13/13	0.89	0.12	41,44,46,47	0
2	MN	B	387	1/1	0.94	0.05	52,52,52,52	0
2	MN	A	387	1/1	0.96	0.07	31,31,31,31	0

6.5 Other polymers

There are no such residues in this entry.