



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:03 AM UTC

PDB ID : 3KSC / pdb_00003ksc
Title : Crystal structure of pea prolegumin, an 11S seed globulin from *Pisum sativum* L.
Authors : Tandang-Silvas, M.R.G.; Fukuda, T.; Fukuda, C.; Prak, K.; Cabanos, C.; Kimura, A.; Itoh, T.; Mikami, B.; Maruyama, N.; Utsumi, S.
Deposited on : 2009-11-21
Resolution : 2.61 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:

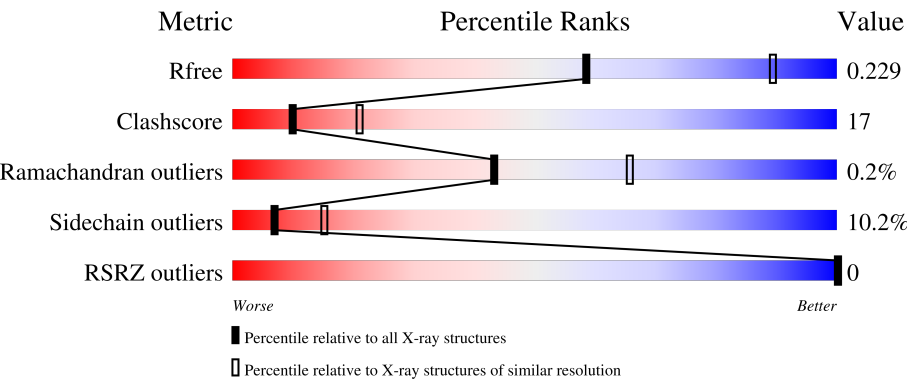
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	496	50% 24% • 23%
1	B	496	49% 26% • 23%
1	C	496	50% 22% • 24%
1	D	496	49% 23% • 24%
1	E	496	51% 23% • 23%

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Mol	Chain	Length	Quality of chain
1	F	496	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	503	-	-	X	-
3	GOL	B	504	-	-	X	-
3	GOL	B	505	-	-	X	-
3	GOL	B	506	-	-	X	-
3	GOL	C	499	-	-	X	-
3	GOL	D	499	-	-	X	-
3	GOL	F	499	-	-	X	-

2 Entry composition [i](#)

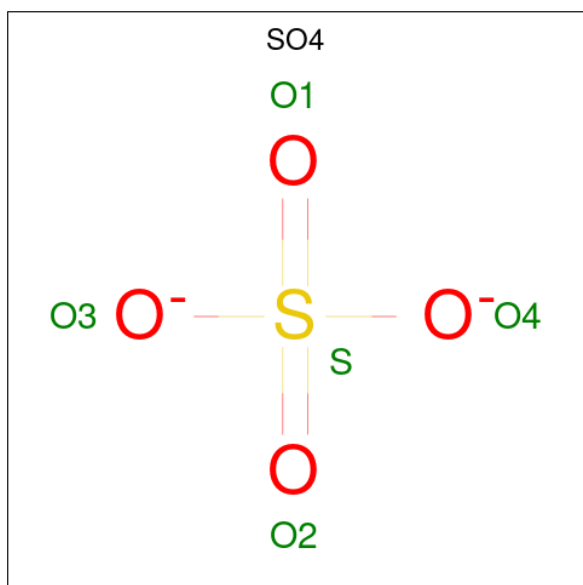
There are 4 unique types of molecules in this entry. The entry contains 18563 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 LegA class.

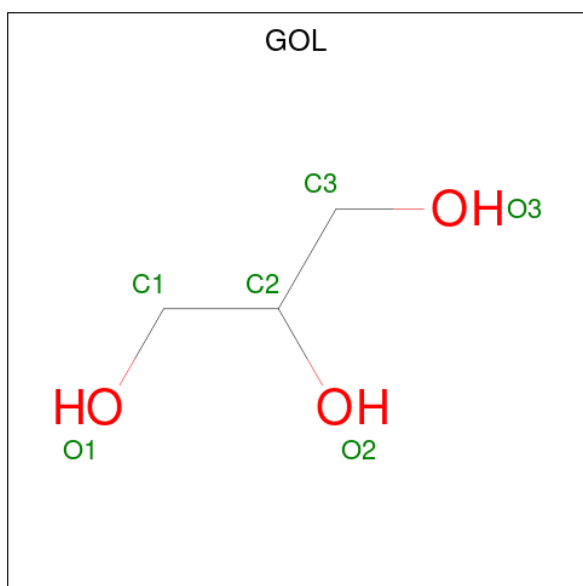
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			3011	1886	556	560	9			
1	B	383	Total	C	N	O	S	0	0	0
			3039	1903	559	568	9			
1	C	375	Total	C	N	O	S	0	0	0
			2967	1859	545	554	9			
1	D	376	Total	C	N	O	S	0	0	0
			2980	1867	548	556	9			
1	E	383	Total	C	N	O	S	0	0	0
			3045	1910	563	563	9			
1	F	377	Total	C	N	O	S	0	2	0
			3007	1883	556	559	9			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0
3	F	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	53	Total O 53 53	0	0
4	B	73	Total O 73 73	0	0

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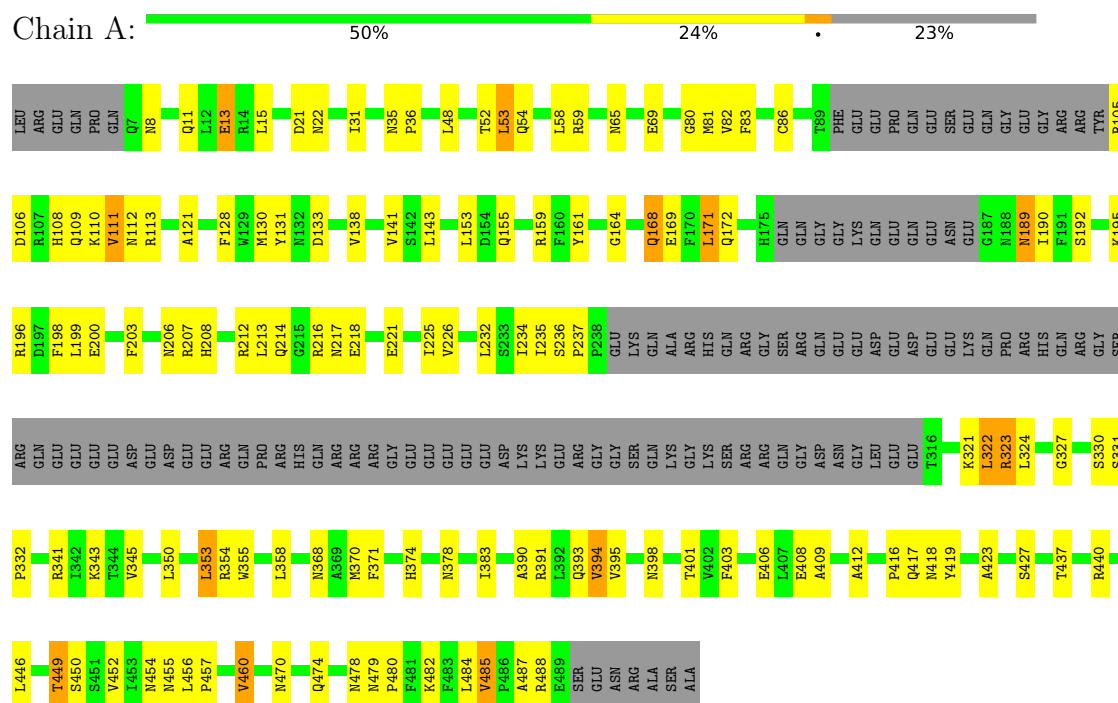
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	62	Total 62	O 62	0	0
4	D	60	Total 60	O 60	0	0
4	E	47	Total 47	O 47	0	0
4	F	46	Total 46	O 46	0	0

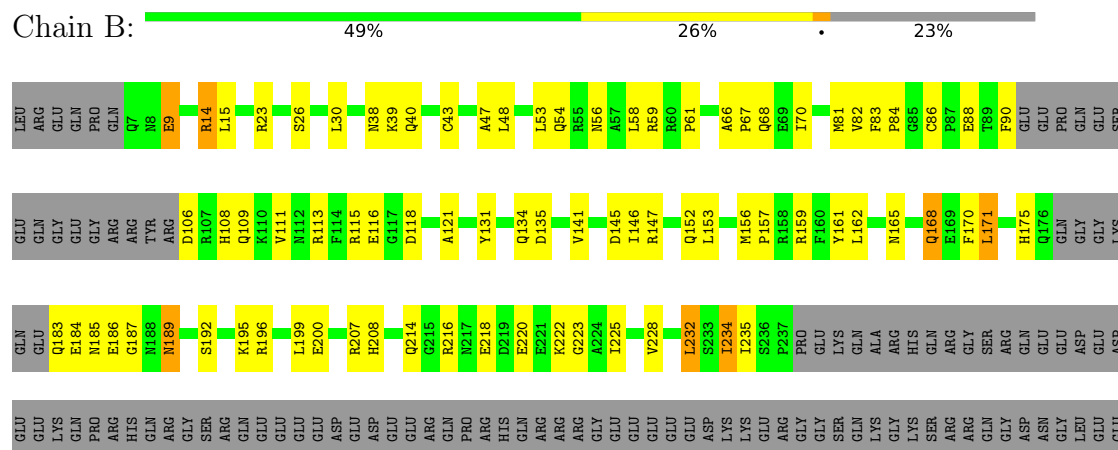
3 Residue-property plots

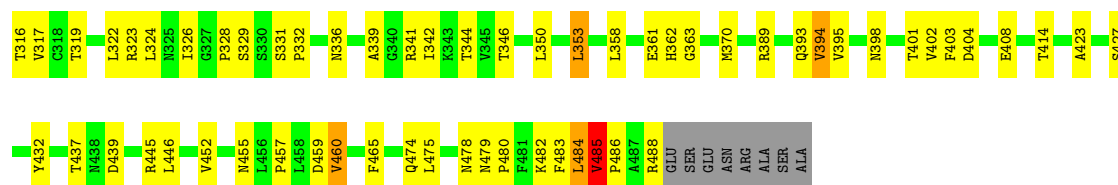
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



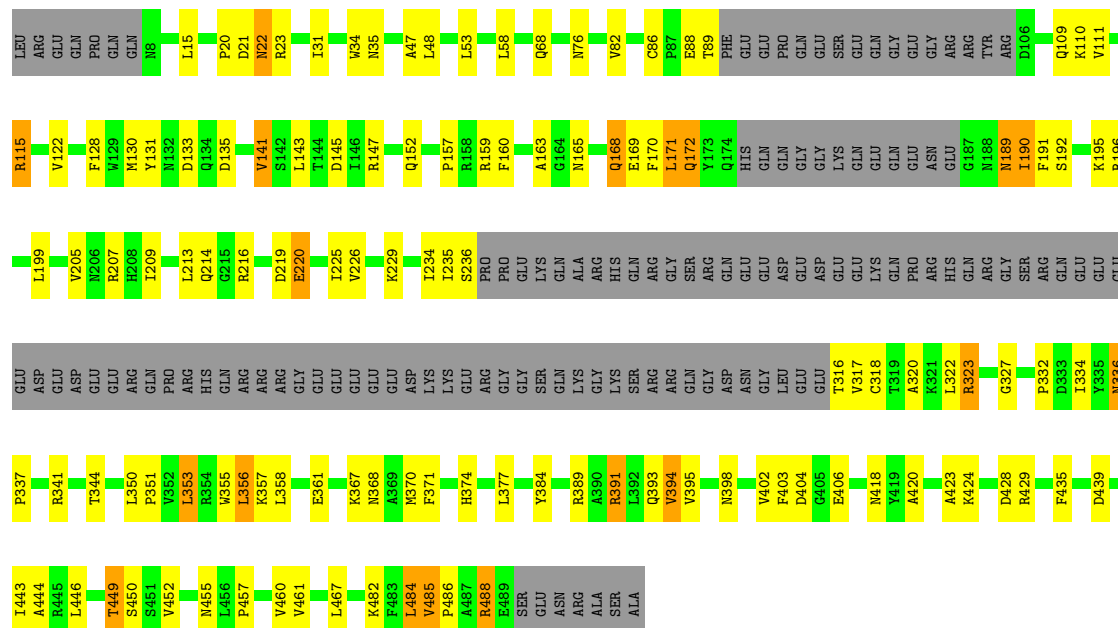
• Molecule 1: LegA class





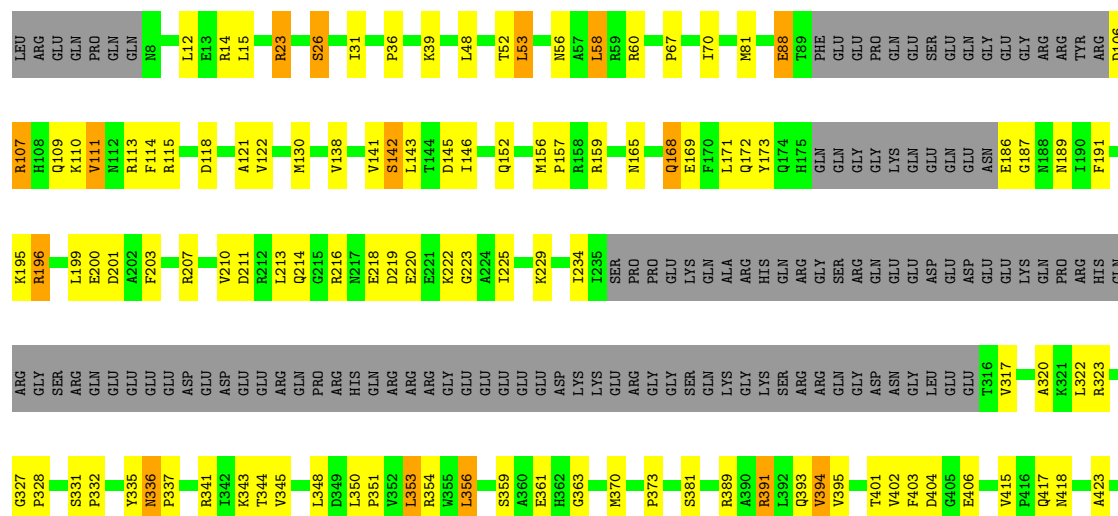
• Molecule 1: LegA class

Chain C: 50% 22% 24%



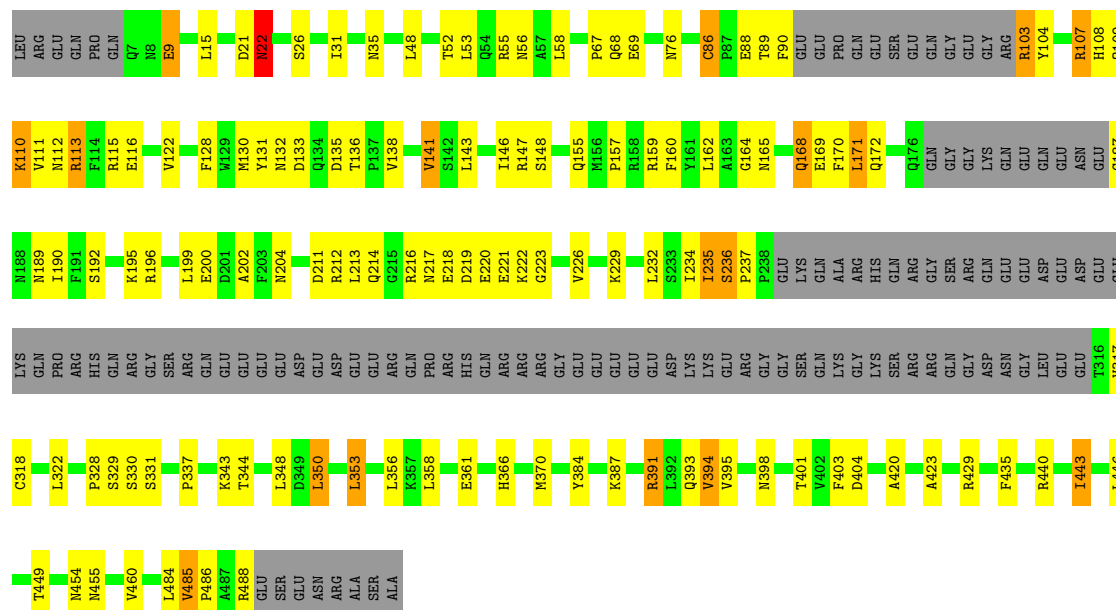
• Molecule 1: LegA class

Chain D: 49% 23% 24%

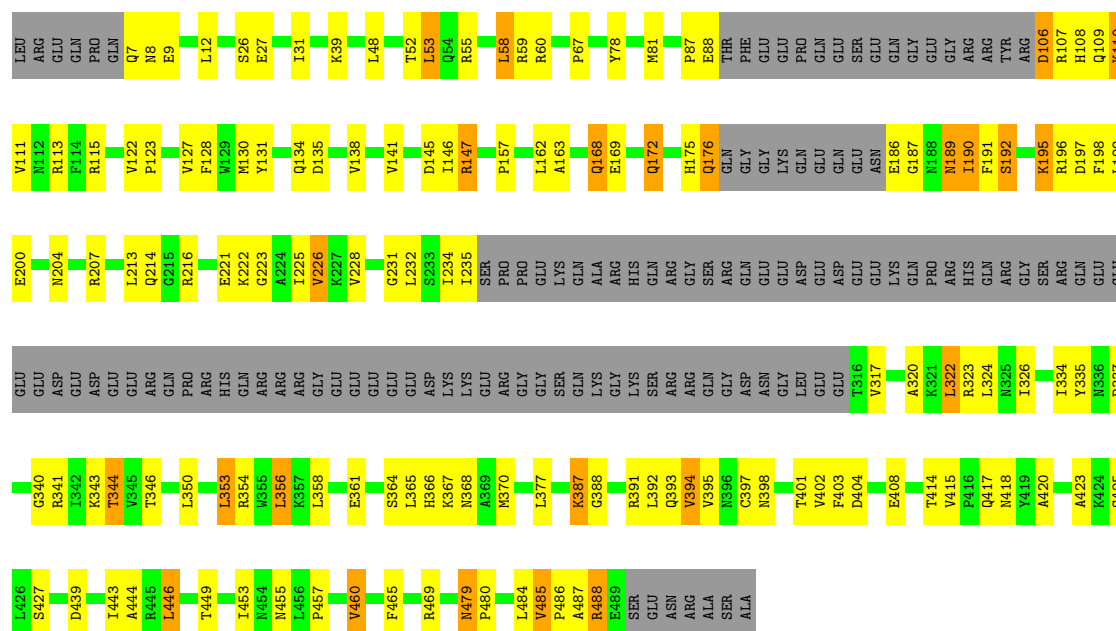




• Molecule 1: LegA class



• Molecule 1: LegA class



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	129.78Å 148.44Å 149.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.06 – 2.61 49.06 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.06-2.61) 99.3 (49.06-2.61)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.175 , 0.234 0.172 , 0.229	Depositor DCC
R_{free} test set	4426 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.069 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18563	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: GOL, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/3070	0.78	2/4155 (0.0%)
1	B	0.41	0/3098	0.79	2/4192 (0.0%)
1	C	0.41	0/3023	0.80	6/4090 (0.1%)
1	D	0.40	0/3037	0.80	7/4109 (0.2%)
1	E	0.41	0/3106	0.80	7/4203 (0.2%)
1	F	0.38	0/3068	0.80	4/4148 (0.1%)
All	All	0.40	0/18402	0.79	28/24897 (0.1%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	336	ASN	CA-C-N	6.80	127.36	119.47
1	C	336	ASN	C-N-CA	6.80	127.36	119.47
1	C	327	GLY	CA-C-N	6.18	126.64	119.47
1	C	327	GLY	C-N-CA	6.18	126.64	119.47
1	F	479	ASN	CA-C-N	6.13	125.83	119.64
1	F	479	ASN	C-N-CA	6.13	125.83	119.64
1	E	350	LEU	CA-C-N	6.00	127.34	119.84
1	E	350	LEU	C-N-CA	6.00	127.34	119.84
1	B	485	VAL	CA-C-N	5.99	125.96	120.03
1	B	485	VAL	C-N-CA	5.99	125.96	120.03
1	D	336	ASN	CA-C-N	5.91	125.61	119.82
1	D	336	ASN	C-N-CA	5.91	125.61	119.82
1	D	479	ASN	CA-C-N	5.68	126.17	120.04
1	D	479	ASN	C-N-CA	5.68	126.17	120.04
1	E	86	CYS	CA-C-N	5.63	125.95	119.93
1	E	86	CYS	C-N-CA	5.63	125.95	119.93
1	C	86	CYS	CA-C-N	5.39	125.39	119.89
1	C	86	CYS	C-N-CA	5.39	125.39	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	415	VAL	CA-C-N	5.32	125.24	119.76
1	F	415	VAL	C-N-CA	5.32	125.24	119.76
1	E	318	CYS	N-CA-C	-5.29	106.84	113.72
1	D	327	GLY	CA-C-N	5.15	124.76	119.56
1	D	327	GLY	C-N-CA	5.15	124.76	119.56
1	D	449	THR	N-CA-C	5.14	116.88	111.28
1	E	449	THR	N-CA-C	5.04	116.78	111.28
1	E	22	ASN	N-CA-C	5.04	116.89	108.99
1	A	327	GLY	CA-C-N	5.02	124.68	119.56
1	A	327	GLY	C-N-CA	5.02	124.68	119.56

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	3011	0	2962	110	0
1	B	3039	0	2979	122	0
1	C	2967	0	2920	116	0
1	D	2980	0	2928	121	0
1	E	3045	0	2995	111	0
1	F	3007	0	2958	114	0
2	A	10	0	0	0	0
2	B	30	0	0	0	0
2	C	10	0	0	0	0
2	D	5	0	0	1	0
2	E	10	0	0	0	0
3	A	12	0	16	2	0
3	B	30	0	40	27	0
3	C	24	0	32	11	0
3	D	18	0	24	8	0
3	E	6	0	8	0	0
3	F	18	0	24	7	0
4	A	53	0	0	9	0
4	B	73	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	62	0	0	1	0
4	D	60	0	0	1	0
4	E	47	0	0	1	0
4	F	46	0	0	3	0
All	All	18563	0	17886	629	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 17.

All (629) 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:E:31:ILE:HG21	1:E:169:GLU:HG2	1.27	1.16
1:F:186:GLU:HG3	1:F:187:GLY:H	1.17	1.08
1:D:391:ARG:HG3	1:D:391:ARG:HH11	1.15	1.04
1:D:328:PRO:HG3	3:D:500:GOL:H31	1.41	1.03
1:F:31:ILE:HG21	1:F:169:GLU:HG2	1.41	1.00
1:D:31:ILE:HG21	1:D:169:GLU:HG2	1.45	0.96
1:C:344:THR:HG22	1:C:361:GLU:HG3	1.48	0.95
1:B:393:GLN:HE22	1:C:195:LYS:H	1.03	0.95
1:D:455:ASN:HD22	1:F:109:GLN:HG3	1.31	0.95
1:A:13:GLU:H	1:A:13:GLU:CD	1.76	0.94
3:B:503:GOL:H2	1:E:115:ARG:HG2	1.48	0.94
1:C:229:LYS:H	1:C:229:LYS:HD2	1.30	0.94
1:B:455:ASN:HD22	1:C:109:GLN:HG3	1.34	0.92
1:E:103:ARG:HH22	1:F:469:ARG:HD2	1.33	0.91
1:C:31:ILE:HG21	1:C:169:GLU:HG2	1.54	0.89
1:A:86:CYS:HB2	1:A:109:GLN:NE2	1.89	0.88
1:D:391:ARG:HH11	1:D:391:ARG:CG	1.86	0.87
1:F:323:ARG:HH12	3:F:498:GOL:H31	1.40	0.86
1:F:195[B]:LYS:HE2	3:F:499:GOL:H31	1.57	0.84
1:E:370:MET:HB2	1:E:423:ALA:O	1.77	0.84
1:D:70:ILE:HG12	1:D:142:SER:HB3	1.57	0.84
1:B:113:ARG:HD3	3:B:503:GOL:H32	1.61	0.83
1:E:350:LEU:HB3	1:E:353:LEU:HD22	1.61	0.82
1:D:393:GLN:HE22	1:F:195[A]:LYS:H	1.26	0.82
1:E:214:GLN:NE2	1:E:216:ARG:HE	1.78	0.82
1:D:393:GLN:HE22	1:F:195[B]:LYS:H	1.27	0.81
1:E:103:ARG:HH12	1:F:469:ARG:HH11	1.26	0.81
1:A:31:ILE:HG21	1:A:169:GLU:HG2	1.62	0.81
1:B:146:ILE:HD11	1:B:157:PRO:HG3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:GLU:HG2	1:E:455:ASN:HD21	1.44	0.80
1:E:214:GLN:HE21	1:E:216:ARG:HE	1.29	0.80
1:A:236:SER:HB2	1:A:237:PRO:HA	1.62	0.79
1:D:130:MET:HE1	1:D:138:VAL:HG11	1.65	0.79
1:F:186:GLU:HG3	1:F:187:GLY:N	1.98	0.79
3:B:504:GOL:H32	1:E:55:ARG:NE	1.98	0.79
1:B:362:HIS:HE1	3:B:504:GOL:H2	1.48	0.78
3:B:504:GOL:H32	1:E:55:ARG:HE	1.48	0.78
1:C:21:ASP:OD2	1:C:35:ASN:HB2	1.83	0.78
1:A:393:GLN:HE22	1:B:195:LYS:H	1.30	0.77
1:B:389:ARG:HD3	3:B:505:GOL:H11	1.64	0.77
1:B:362:HIS:CE1	3:B:504:GOL:H2	2.20	0.77
1:B:328:PRO:HG3	3:B:504:GOL:H11	1.66	0.76
1:D:31:ILE:CG2	1:D:169:GLU:HG2	2.15	0.76
1:B:228:VAL:HG11	1:B:232:LEU:HD23	1.68	0.75
1:D:196:ARG:HE	1:D:207:ARG:HE	1.32	0.75
1:D:67:PRO:HG2	1:D:145:ASP:HB3	1.67	0.75
1:B:165:ASN:OD1	1:B:187:GLY:HA2	1.86	0.75
1:F:370:MET:HB2	1:F:423:ALA:O	1.86	0.75
1:A:332:PRO:HG3	1:A:341:ARG:NH2	2.02	0.74
1:D:88:GLU:HG2	1:E:455:ASN:ND2	2.02	0.73
1:D:389:ARG:HH21	3:D:499:GOL:H12	1.51	0.73
1:A:212:ARG:HH12	1:A:217:ASN:HD22	1.37	0.73
1:E:344:THR:HG22	1:E:361:GLU:HG3	1.69	0.73
1:F:214:GLN:NE2	1:F:216:ARG:HE	1.86	0.72
1:C:370:MET:HB2	1:C:423:ALA:O	1.90	0.71
1:E:236:SER:H	1:E:237:PRO:CD	2.03	0.71
1:A:394:VAL:HG13	1:A:403:PHE:HB3	1.72	0.71
1:B:214:GLN:NE2	1:B:216:ARG:HE	1.89	0.71
1:D:391:ARG:HG3	1:D:391:ARG:NH1	1.96	0.70
1:C:214:GLN:NE2	1:C:216:ARG:HE	1.89	0.70
1:B:370:MET:HB2	1:B:423:ALA:O	1.92	0.70
1:C:68:GLN:HE21	1:C:159:ARG:HH21	1.37	0.69
3:B:503:GOL:C2	1:E:115:ARG:HG2	2.21	0.69
1:B:196:ARG:HD2	1:B:207:ARG:NE	2.06	0.69
1:C:323:ARG:HH22	3:C:501:GOL:H2	1.55	0.69
1:D:196:ARG:HG3	1:D:210:VAL:HG11	1.75	0.69
1:D:344:THR:HG22	1:D:361:GLU:HG3	1.75	0.69
1:E:236:SER:H	1:E:237:PRO:HD2	1.58	0.69
1:A:53:LEU:HD22	1:A:225:ILE:HD13	1.73	0.69
1:C:394:VAL:HG13	1:C:403:PHE:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:394:VAL:HG13	1:F:403:PHE:HB3	1.75	0.68
1:C:449:THR:HB	1:C:482:LYS:HA	1.76	0.68
1:E:76:ASN:HD22	1:E:115:ARG:HA	1.57	0.68
1:A:398:ASN:ND2	1:B:171:LEU:HG	2.09	0.68
1:B:394:VAL:HG13	1:B:403:PHE:HB3	1.76	0.68
1:C:374:HIS:NE2	3:C:500:GOL:H2	2.09	0.68
1:B:393:GLN:HE22	1:C:195:LYS:N	1.85	0.68
1:B:457:PRO:HB2	1:B:460:VAL:HG13	1.74	0.67
1:B:196:ARG:NH1	1:B:207:ARG:HE	1.90	0.67
1:C:229:LYS:HD2	1:C:229:LYS:N	2.08	0.67
1:A:86:CYS:HB2	1:A:109:GLN:HE22	1.58	0.67
1:B:353:LEU:HG	1:B:358:LEU:O	1.94	0.67
1:D:109:GLN:HG3	1:E:455:ASN:HD22	1.59	0.67
1:F:189:ASN:ND2	1:F:192:SER:H	1.91	0.67
1:C:229:LYS:H	1:C:229:LYS:CD	2.07	0.67
1:E:22:ASN:CG	1:E:172:GLN:HE22	2.03	0.66
1:F:67:PRO:HG2	1:F:145:ASP:HB3	1.76	0.66
1:A:105:ARG:N	1:A:106:ASP:HA	2.10	0.66
1:B:196:ARG:HH11	1:B:207:ARG:HE	1.43	0.66
1:E:110:LYS:HE3	1:E:112:ASN:HD21	1.61	0.66
3:B:507:GOL:H2	1:E:429:ARG:NH1	2.11	0.66
1:F:172:GLN:HG2	4:F:508:HOH:O	1.95	0.66
1:F:195[A]:LYS:HE2	3:F:499:GOL:O3	1.96	0.66
1:B:401:THR:HG21	1:B:404:ASP:HB2	1.77	0.65
1:D:391:ARG:HH21	3:F:499:GOL:H32	1.59	0.65
1:F:162:LEU:HA	1:F:190:ILE:HD11	1.78	0.65
1:B:187:GLY:HA3	4:B:548:HOH:O	1.97	0.65
1:D:195:LYS:HD2	1:E:391:ARG:HH21	1.60	0.65
3:B:507:GOL:O3	1:E:387:LYS:HE2	1.96	0.65
1:A:460:VAL:HG12	1:B:232:LEU:HD11	1.78	0.65
4:A:548:HOH:O	1:B:208:HIS:HE1	1.79	0.65
1:C:207:ARG:HE	3:C:502:GOL:H32	1.61	0.64
1:B:168:GLN:OE1	1:B:170:PHE:HB2	1.97	0.64
1:C:370:MET:HG3	1:C:485:VAL:HG13	1.78	0.63
3:B:503:GOL:H2	1:E:115:ARG:CG	2.26	0.63
1:B:108:HIS:HD2	1:B:109:GLN:O	1.82	0.63
1:E:103:ARG:HH12	1:F:469:ARG:NH1	1.96	0.63
1:B:401:THR:CG2	1:B:404:ASP:HB2	2.29	0.63
1:E:165:ASN:OD1	1:E:187:GLY:HA2	1.99	0.63
1:A:212:ARG:NH1	1:A:217:ASN:HD22	1.95	0.63
1:C:391:ARG:NH1	1:C:404:ASP:OD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:GLN:HE22	1:E:216:ARG:HH11	1.46	0.63
1:F:350:LEU:HB3	1:F:353:LEU:HD22	1.79	0.63
1:F:353:LEU:HG	1:F:358:LEU:O	1.99	0.63
1:D:15:LEU:HB2	1:D:403:PHE:HB2	1.81	0.63
1:C:323:ARG:HH11	1:C:323:ARG:HB3	1.64	0.62
1:A:15:LEU:HB2	1:A:403:PHE:HB2	1.82	0.62
1:A:321:LYS:HE2	1:A:323:ARG:O	2.00	0.62
1:B:118:ASP:OD2	1:B:323:ARG:HD2	2.00	0.61
1:E:143:LEU:HD13	1:E:435:PHE:CB	2.31	0.61
1:A:189:ASN:HD22	1:A:189:ASN:C	2.09	0.61
1:B:59:ARG:HH21	3:B:506:GOL:H31	1.64	0.61
1:D:348:LEU:HD21	1:D:440:ARG:NH1	2.15	0.61
1:B:115:ARG:HG2	4:B:529:HOH:O	2.01	0.61
1:A:457:PRO:HB2	1:A:460:VAL:HG13	1.83	0.61
1:C:207:ARG:NE	3:C:502:GOL:H32	2.15	0.61
1:D:317:VAL:HG22	1:D:320:ALA:HB2	1.83	0.60
1:E:162:LEU:HD22	1:E:190:ILE:HD11	1.83	0.60
1:A:393:GLN:OE1	1:B:195:LYS:HG2	2.00	0.60
1:D:370:MET:HG3	1:D:485:VAL:HG13	1.83	0.60
1:C:234:ILE:HG22	1:C:236:SER:H	1.65	0.60
1:D:363:GLY:HA3	1:D:432:TYR:CZ	2.36	0.60
1:F:370:MET:HG3	1:F:485:VAL:HG13	1.84	0.60
1:D:26:SER:HB3	1:D:223:GLY:HA3	1.84	0.60
1:A:195:LYS:HG3	4:A:509:HOH:O	2.01	0.60
1:B:445:ARG:NH2	1:B:482:LYS:HE2	2.17	0.60
1:D:331:SER:O	1:D:343:LYS:HE2	2.02	0.60
1:A:108:HIS:HD2	1:A:109:GLN:O	1.85	0.60
1:C:15:LEU:HB2	1:C:403:PHE:HB2	1.84	0.60
1:F:370:MET:CB	1:F:423:ALA:O	2.50	0.60
1:B:161:TYR:HE1	4:B:562:HOH:O	1.84	0.59
1:C:323:ARG:HB3	1:C:323:ARG:NH1	2.17	0.59
1:D:214:GLN:HE21	1:D:216:ARG:HE	1.50	0.59
1:C:168:GLN:OE1	1:C:170:PHE:HB2	2.00	0.59
1:C:393:GLN:HG2	1:C:404:ASP:OD1	2.02	0.59
1:F:88:GLU:HB3	1:F:108:HIS:O	2.01	0.59
1:E:443:ILE:HG13	1:E:443:ILE:O	1.99	0.59
1:A:131:TYR:CE2	1:A:133:ASP:HB3	2.39	0.58
1:E:31:ILE:CG2	1:E:169:GLU:HG2	2.18	0.58
1:A:22:ASN:CG	1:A:172:GLN:HE22	2.11	0.58
1:A:440:ARG:NH2	1:B:316:THR:HG23	2.19	0.58
1:A:13:GLU:CD	1:A:13:GLU:N	2.53	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:GLU:OE2	1:D:207:ARG:HD3	2.04	0.57
1:E:212:ARG:NH1	1:E:217:ASN:HD22	2.03	0.57
1:C:449:THR:HG22	1:C:450:SER:N	2.19	0.57
1:D:196:ARG:HG3	1:D:210:VAL:CG1	2.34	0.57
1:A:455:ASN:HB3	1:B:109:GLN:HG3	1.86	0.57
1:B:362:HIS:CE1	3:B:504:GOL:H12	2.40	0.57
1:C:76:ASN:ND2	1:C:115:ARG:HB3	2.19	0.57
1:A:371:PHE:CE1	1:A:374:HIS:HE1	2.21	0.57
1:B:189:ASN:C	1:B:189:ASN:HD22	2.13	0.57
1:E:353:LEU:HG	1:E:358:LEU:O	2.05	0.57
1:A:189:ASN:ND2	1:A:192:SER:H	2.03	0.57
1:A:350:LEU:HB3	1:A:353:LEU:HD22	1.86	0.57
1:B:344:THR:HG22	1:B:361:GLU:HG3	1.87	0.57
1:D:58:LEU:HD13	1:D:60:ARG:HG2	1.87	0.57
1:A:196:ARG:HD2	1:A:207:ARG:HD2	1.87	0.56
1:C:361:GLU:OE2	3:C:500:GOL:O1	2.22	0.56
1:C:189:ASN:ND2	1:C:192:SER:H	2.03	0.56
1:D:53:LEU:HD11	1:D:130:MET:HE2	1.87	0.56
1:A:427:SER:HB3	3:A:500:GOL:H2	1.86	0.56
1:B:218:GLU:HG3	1:B:222:LYS:HD2	1.88	0.56
1:B:70:ILE:HD13	3:B:506:GOL:H12	1.88	0.56
1:E:195:LYS:H	1:F:393:GLN:HE22	1.52	0.56
1:E:370:MET:CB	1:E:423:ALA:O	2.53	0.56
1:F:59:ARG:HD2	4:F:524:HOH:O	2.06	0.56
1:D:159:ARG:HB2	1:D:168:GLN:HG3	1.89	0.55
1:E:143:LEU:HD13	1:E:435:PHE:HB2	1.89	0.55
1:E:214:GLN:HE21	1:E:216:ARG:NE	2.02	0.55
1:B:200:GLU:OE2	1:B:207:ARG:HD3	2.06	0.55
1:F:58:LEU:HB3	1:F:226:VAL:HG12	1.89	0.55
1:B:329:SER:HB2	4:E:540:HOH:O	2.06	0.55
1:D:107:ARG:H	1:D:107:ARG:NH2	2.04	0.55
1:B:389:ARG:HG2	1:B:408:GLU:HB2	1.88	0.55
1:B:455:ASN:ND2	1:C:109:GLN:HG3	2.13	0.55
1:C:370:MET:CB	1:C:423:ALA:O	2.55	0.55
1:F:340:GLY:HA3	1:F:364:SER:O	2.05	0.55
1:A:200:GLU:OE2	1:A:207:ARG:HD3	2.06	0.55
1:E:214:GLN:NE2	1:E:216:ARG:NE	2.54	0.55
1:F:53:LEU:HD22	1:F:225:ILE:HD13	1.88	0.55
1:A:427:SER:CB	3:A:500:GOL:H2	2.36	0.55
1:B:40:GLN:HE21	1:B:414:THR:H	1.53	0.55
1:B:336:ASN:HB3	1:B:339:ALA:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ASN:CG	1:C:172:GLN:HE22	2.15	0.55
1:F:26:SER:HB2	1:F:223:GLY:HA3	1.89	0.55
1:F:189:ASN:HD22	1:F:189:ASN:C	2.14	0.55
1:F:346:THR:HB	1:F:439:ASP:O	2.06	0.55
1:D:478:ASN:HB3	1:F:204:ASN:HB3	1.90	0.54
1:E:131:TYR:CG	1:E:232:LEU:HD12	2.43	0.54
1:D:81:MET:HE1	1:D:121:ALA:O	2.07	0.54
1:D:391:ARG:CG	1:D:391:ARG:NH1	2.56	0.54
1:A:370:MET:HB2	1:A:423:ALA:O	2.06	0.54
1:B:113:ARG:CD	3:B:503:GOL:H32	2.36	0.54
1:B:183:GLN:OE1	1:B:185:ASN:HB3	2.07	0.54
1:E:90:PHE:CD1	1:E:90:PHE:C	2.85	0.54
1:A:111:VAL:HG11	1:A:234:ILE:HG22	1.90	0.54
1:A:370:MET:HG3	1:A:485:VAL:HG13	1.89	0.54
1:E:15:LEU:HB2	1:E:403:PHE:HB2	1.88	0.54
1:F:427:SER:OG	3:F:497:GOL:H2	2.07	0.54
1:A:169:GLU:HG3	4:A:542:HOH:O	2.07	0.54
1:D:348:LEU:HD11	1:D:440:ARG:NH2	2.23	0.54
1:E:196:ARG:HD3	1:E:211:ASP:OD1	2.08	0.54
1:D:196:ARG:NH2	1:D:216:ARG:NH1	2.56	0.54
1:D:332:PRO:HG3	1:D:341:ARG:CZ	2.38	0.53
1:B:134:GLN:NE2	1:E:115:ARG:HE	2.07	0.53
1:D:196:ARG:NE	1:D:207:ARG:HE	2.03	0.53
1:B:26:SER:HB3	1:B:223:GLY:HA3	1.90	0.53
1:C:131:TYR:CE2	1:C:133:ASP:HB3	2.43	0.53
1:D:370:MET:CB	1:D:423:ALA:O	2.56	0.53
1:C:68:GLN:NE2	1:C:159:ARG:HH21	2.05	0.53
1:D:417:GLN:O	1:D:418:ASN:HB2	2.08	0.53
1:F:370:MET:CG	1:F:485:VAL:HG13	2.39	0.53
1:B:362:HIS:CE1	3:B:504:GOL:C2	2.91	0.53
1:E:159:ARG:HB2	1:E:168:GLN:HG3	1.90	0.53
1:B:9:GLU:O	1:B:43:CYS:HB2	2.09	0.53
1:D:458:LEU:HB2	1:F:106:ASP:HB3	1.90	0.53
1:C:351:PRO:HB2	3:C:499:GOL:H11	1.90	0.52
1:E:88:GLU:OE1	1:E:107:ARG:HD2	2.09	0.52
1:E:164:GLY:HA2	1:E:218:GLU:OE1	2.09	0.52
1:F:222:LYS:HE3	1:F:226:VAL:CG2	2.39	0.52
1:A:368:ASN:C	1:A:487:ALA:HB2	2.34	0.52
1:E:109:GLN:HG3	1:F:455:ASN:HD22	1.74	0.52
1:E:168:GLN:HG2	1:E:170:PHE:H	1.74	0.52
1:E:213:LEU:HD12	1:F:465:PHE:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LEU:HD22	1:C:225:ILE:HG21	1.91	0.52
1:D:143:LEU:C	1:D:143:LEU:HD23	2.34	0.52
1:B:427:SER:HB3	3:B:505:GOL:H32	1.92	0.52
1:E:219:ASP:OD1	1:E:221:GLU:HB2	2.10	0.52
1:F:55[B]:ARG:HG3	1:F:134:GLN:O	2.10	0.52
1:F:457:PRO:HB2	1:F:460:VAL:HG13	1.92	0.52
1:B:189:ASN:ND2	1:B:192:SER:H	2.08	0.52
1:C:131:TYR:HE2	1:C:133:ASP:HB3	1.73	0.52
1:D:200:GLU:HG3	1:D:210:VAL:HG21	1.91	0.52
1:D:111:VAL:HG21	1:D:234:ILE:HG21	1.92	0.51
1:A:437:THR:OG1	1:B:152:GLN:NE2	2.43	0.51
1:B:350:LEU:HB3	1:B:353:LEU:HD22	1.92	0.51
1:D:214:GLN:NE2	1:D:216:ARG:HE	2.08	0.51
1:A:159:ARG:HB2	1:A:168:GLN:HG3	1.92	0.51
1:C:207:ARG:HE	3:C:502:GOL:C3	2.23	0.51
1:E:26:SER:HB3	1:E:223:GLY:HA3	1.92	0.51
1:A:206:ASN:OD1	1:A:208:HIS:HB3	2.11	0.51
1:B:474:GLN:HE21	1:B:478:ASN:HD21	1.58	0.51
1:F:88:GLU:OE2	1:F:107:ARG:HB3	2.10	0.51
1:F:195[B]:LYS:HE2	3:F:499:GOL:C3	2.35	0.51
1:A:189:ASN:HD22	1:A:192:SER:H	1.58	0.51
1:A:330:SER:HB2	1:A:343:LYS:HE2	1.92	0.51
1:A:341:ARG:HD2	4:A:512:HOH:O	2.10	0.51
1:C:190:ILE:HD12	1:C:191:PHE:N	2.26	0.51
1:D:118:ASP:OD2	1:D:323:ARG:HD2	2.11	0.51
1:D:370:MET:HG3	1:D:485:VAL:CG1	2.40	0.51
1:F:195[B]:LYS:O	1:F:198:PHE:HB2	2.11	0.51
1:A:164:GLY:HA2	1:A:218:GLU:OE1	2.10	0.51
1:E:103:ARG:NH2	1:F:469:ARG:HD2	2.15	0.51
1:F:131:TYR:CG	1:F:232:LEU:HD12	2.46	0.51
1:B:131:TYR:CZ	1:B:232:LEU:HB2	2.47	0.50
1:E:236:SER:N	1:E:237:PRO:CD	2.73	0.50
1:A:54:GLN:HG3	4:A:537:HOH:O	2.10	0.50
1:A:378:ASN:HA	1:A:417:GLN:NE2	2.27	0.50
1:C:220:GLU:CD	1:C:220:GLU:H	2.19	0.50
1:C:334:ILE:CD1	1:C:482:LYS:HG2	2.42	0.50
1:E:68:GLN:HB2	1:E:122:VAL:HB	1.94	0.50
1:A:455:ASN:ND2	1:B:109:GLN:HG3	2.26	0.50
1:D:106:ASP:HA	1:D:107:ARG:NH2	2.26	0.50
1:C:189:ASN:C	1:C:189:ASN:HD22	2.19	0.50
1:D:12:LEU:HD23	1:D:39:LYS:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ARG:HG3	1:C:147:ARG:HH11	1.77	0.50
1:C:159:ARG:O	1:C:168:GLN:HG3	2.11	0.50
1:D:23:ARG:HG2	1:D:23:ARG:HH11	1.76	0.50
1:F:228:VAL:HG12	1:F:231:GLY:H	1.77	0.50
1:A:390:ALA:O	1:A:406:GLU:HA	2.11	0.50
1:B:67:PRO:HG2	1:B:145:ASP:HB3	1.93	0.50
1:A:214:GLN:HE22	1:A:216:ARG:HH11	1.60	0.49
1:A:113:ARG:HH21	1:A:113:ARG:HB3	1.76	0.49
1:A:59:ARG:HB3	1:A:130:MET:HB2	1.95	0.49
1:B:38:ASN:ND2	4:B:546:HOH:O	2.45	0.49
1:C:334:ILE:HD11	1:C:482:LYS:HG2	1.94	0.49
1:B:362:HIS:HE1	3:B:504:GOL:C2	2.23	0.49
1:C:31:ILE:HG21	1:C:169:GLU:CG	2.33	0.49
1:F:394:VAL:HA	1:F:420:ALA:O	2.11	0.49
1:B:90:PHE:CD1	1:B:90:PHE:C	2.90	0.49
1:B:156:MET:HE3	1:B:157:PRO:HD2	1.95	0.49
1:D:393:GLN:NE2	1:F:195[A]:LYS:H	2.01	0.49
1:E:235:ILE:HD13	1:E:235:ILE:H	1.78	0.49
1:F:350:LEU:O	1:F:353:LEU:HB2	2.12	0.49
1:A:81:MET:HE1	1:A:121:ALA:O	2.12	0.49
1:B:452:VAL:HA	1:C:82:VAL:HG11	1.94	0.49
1:C:394:VAL:HG22	1:C:402:VAL:CG2	2.42	0.49
1:D:109:GLN:HG3	1:E:455:ASN:ND2	2.26	0.49
1:F:195[A]:LYS:HD3	1:F:197:ASP:HB2	1.94	0.49
1:F:190:ILE:HD12	1:F:191:PHE:H	1.78	0.49
1:F:487:ALA:HA	1:F:488:ARG:NH1	2.28	0.49
1:A:83:PHE:HE2	1:A:322:LEU:HD21	1.78	0.48
1:F:189:ASN:ND2	1:F:192:SER:N	2.61	0.48
1:D:393:GLN:NE2	1:F:195[B]:LYS:H	2.03	0.48
1:E:165:ASN:O	1:E:220:GLU:HG2	2.13	0.48
1:F:326:ILE:HA	1:F:343:LYS:HD2	1.95	0.48
1:E:113:ARG:HG3	1:E:237:PRO:HG2	1.95	0.48
1:A:195:LYS:HD2	1:C:391:ARG:NH2	2.29	0.48
1:B:393:GLN:OE1	1:C:195:LYS:HG3	2.14	0.48
1:B:394:VAL:HG22	1:B:402:VAL:CG2	2.44	0.48
1:D:458:LEU:HB2	1:F:106:ASP:CB	2.44	0.48
1:F:123:PRO:HA	1:F:356:LEU:HD22	1.95	0.48
1:F:128:PHE:CZ	1:F:130:MET:HG3	2.48	0.48
1:F:387:LYS:HG3	1:F:388:GLY:N	2.29	0.48
1:B:81:MET:HE1	1:B:121:ALA:O	2.14	0.48
1:D:195:LYS:HD2	1:E:391:ARG:NH2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:GLY:HA3	1:D:432:TYR:CE1	2.49	0.48
1:B:232:LEU:HD12	1:B:234:ILE:HD13	1.96	0.48
1:A:324:LEU:HD22	1:A:345:VAL:HG23	1.94	0.48
1:B:483:PHE:HD2	1:B:484:LEU:HD13	1.79	0.48
1:C:128:PHE:CZ	1:C:130:MET:HG3	2.49	0.48
1:D:335:TYR:HD1	1:D:341:ARG:HB3	1.79	0.48
1:A:53:LEU:N	1:A:53:LEU:HD23	2.29	0.47
1:D:111:VAL:HG21	1:D:234:ILE:CG2	2.44	0.47
1:E:189:ASN:ND2	1:E:192:SER:H	2.12	0.47
1:A:455:ASN:ND2	1:B:88:GLU:HG2	2.29	0.47
1:B:23:ARG:HB3	1:B:30:LEU:HD11	1.96	0.47
1:F:78:TYR:CZ	1:F:113:ARG:NH1	2.82	0.47
1:B:342:ILE:HD11	1:B:484:LEU:HD11	1.94	0.47
1:E:103:ARG:CG	1:E:104:TYR:H	2.27	0.47
1:B:68:GLN:NE2	1:B:159:ARG:HH21	2.12	0.47
1:B:317:VAL:HG13	1:B:319:THR:HG22	1.95	0.47
1:B:363:GLY:HA3	1:B:432:TYR:CZ	2.49	0.47
1:A:52:THR:HA	1:A:138:VAL:O	2.14	0.47
1:D:146:ILE:HD11	1:D:157:PRO:HD3	1.95	0.47
1:C:374:HIS:O	1:C:420:ALA:HA	2.15	0.47
1:D:56:ASN:ND2	4:D:516:HOH:O	2.48	0.47
1:E:348:LEU:HD11	1:E:440:ARG:NH2	2.30	0.47
1:F:145:ASP:OD1	1:F:147:ARG:HG2	2.14	0.47
1:A:110:LYS:HG2	1:A:112:ASN:OD1	2.15	0.47
1:A:198:PHE:CD2	1:C:393:GLN:NE2	2.81	0.47
1:D:394:VAL:HG22	1:D:402:VAL:HG23	1.95	0.47
1:F:367:LYS:O	1:F:368:ASN:HB2	2.15	0.47
1:A:161:TYR:HE1	4:A:517:HOH:O	1.98	0.47
1:B:232:LEU:HD22	1:B:232:LEU:HA	1.81	0.47
1:C:320:ALA:HA	3:C:499:GOL:H12	1.95	0.47
1:C:393:GLN:HA	1:C:403:PHE:O	2.14	0.47
1:D:479:ASN:HA	1:D:480:PRO:HD3	1.69	0.47
1:B:326:ILE:HD12	1:B:362:HIS:HB2	1.97	0.47
1:B:485:VAL:HA	1:B:486:PRO:HD3	1.73	0.47
1:D:195:LYS:HB2	1:E:393:GLN:HE22	1.80	0.47
1:E:67:PRO:HB3	1:E:356:LEU:HG	1.96	0.47
1:A:479:ASN:HA	1:A:480:PRO:HD3	1.69	0.46
1:B:59:ARG:NH2	3:B:506:GOL:H31	2.30	0.46
1:C:320:ALA:HA	3:C:499:GOL:H2	1.97	0.46
1:C:68:GLN:HE21	1:C:159:ARG:NH2	2.11	0.46
1:D:168:GLN:HG2	1:D:169:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ARG:HD2	1:D:107:ARG:O	2.16	0.46
1:D:370:MET:HB2	1:D:423:ALA:O	2.14	0.46
1:D:143:LEU:HD13	1:D:435:PHE:HB3	1.97	0.46
1:F:12:LEU:CD2	1:F:39:LYS:HD3	2.45	0.46
1:A:378:ASN:HA	1:A:417:GLN:HE21	1.81	0.46
1:E:344:THR:HG22	1:E:361:GLU:CG	2.44	0.46
1:F:323:ARG:HG2	1:F:324:LEU:N	2.30	0.46
1:A:416:PRO:HB2	1:A:419:TYR:CD1	2.50	0.46
1:C:368:ASN:HD22	1:C:424:LYS:HE2	1.80	0.46
1:B:196:ARG:HD2	1:B:207:ARG:HE	1.78	0.46
1:D:389:ARG:HE	3:D:499:GOL:C1	2.28	0.46
1:E:76:ASN:ND2	1:E:115:ARG:HA	2.29	0.46
1:F:12:LEU:HD23	1:F:39:LYS:HD3	1.98	0.46
1:F:81:MET:HE2	1:F:122:VAL:HG22	1.98	0.46
1:E:90:PHE:HD2	1:E:108:HIS:HE1	1.63	0.46
1:C:353:LEU:HG	1:C:358:LEU:O	2.16	0.46
1:D:114:PHE:CZ	1:D:130:MET:HE3	2.51	0.46
1:D:203:PHE:CE2	1:D:213:LEU:HD21	2.51	0.46
1:D:389:ARG:NH2	3:D:499:GOL:H12	2.26	0.46
1:E:350:LEU:O	1:E:353:LEU:HB2	2.16	0.46
1:B:26:SER:CB	1:B:223:GLY:HA3	2.46	0.45
1:F:401:THR:HG21	1:F:404:ASP:HB2	1.98	0.45
1:A:232:LEU:O	1:A:234:ILE:HG13	2.16	0.45
1:A:172:GLN:HG2	4:A:536:HOH:O	2.16	0.45
1:C:219:ASP:OD1	1:C:219:ASP:N	2.49	0.45
1:C:332:PRO:HG3	1:C:341:ARG:NH1	2.32	0.45
1:D:23:ARG:HG2	1:D:23:ARG:NH1	2.31	0.45
1:A:69:GLU:HB2	1:A:358:LEU:HD13	1.97	0.45
3:B:503:GOL:H11	4:B:529:HOH:O	2.16	0.45
1:D:389:ARG:HD2	1:D:406:GLU:OE2	2.17	0.45
1:A:8:ASN:HD21	1:B:156:MET:HG3	1.82	0.45
1:B:56:ASN:ND2	1:E:328:PRO:HB2	2.31	0.45
1:E:88:GLU:HB2	1:E:107:ARG:HD3	1.98	0.45
1:B:14:ARG:HG2	1:B:15:LEU:N	2.31	0.45
1:F:176:GLN:CD	1:F:176:GLN:H	2.24	0.45
1:B:116:GLU:OE2	1:E:136:THR:OG1	2.29	0.45
1:C:20:PRO:HG3	1:C:34:TRP:CH2	2.52	0.45
1:C:370:MET:HG3	1:C:485:VAL:CG1	2.45	0.45
1:C:377:LEU:HD11	1:C:444:ALA:HB2	1.98	0.45
1:F:394:VAL:HG22	1:F:402:VAL:CG2	2.46	0.45
1:C:356:LEU:HD23	1:C:356:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:ARG:HH22	1:E:133:ASP:CG	2.24	0.45
1:E:370:MET:CG	1:E:485:VAL:HG13	2.47	0.45
1:B:370:MET:CB	1:B:423:ALA:O	2.63	0.45
1:D:427:SER:HA	3:D:499:GOL:H32	1.98	0.45
1:E:401:THR:CG2	1:E:404:ASP:HB2	2.46	0.45
1:E:485:VAL:HA	1:E:486:PRO:HD3	1.82	0.45
1:F:53:LEU:N	1:F:53:LEU:HD23	2.32	0.45
1:F:394:VAL:HG22	1:F:402:VAL:HG23	1.98	0.45
1:A:65:ASN:HA	1:C:418:ASN:OD1	2.17	0.45
1:A:196:ARG:O	1:A:200:GLU:HG3	2.16	0.45
1:A:452:VAL:O	1:A:456:LEU:HG	2.17	0.45
1:D:107:ARG:H	1:D:107:ARG:CZ	2.30	0.45
1:F:479:ASN:HA	1:F:480:PRO:HD3	1.70	0.45
1:C:21:ASP:C	1:C:21:ASP:OD1	2.61	0.44
1:C:389:ARG:HD2	1:C:406:GLU:OE2	2.17	0.44
1:F:52:THR:HA	1:F:138:VAL:O	2.17	0.44
1:F:322:LEU:HD13	1:F:322:LEU:HA	1.76	0.44
1:D:36:PRO:HD2	1:D:173:TYR:CD1	2.52	0.44
1:D:317:VAL:HG13	1:D:317:VAL:O	2.17	0.44
1:B:61:PRO:HB2	1:B:162:LEU:HD12	1.99	0.44
1:B:479:ASN:HA	1:B:480:PRO:HD3	1.77	0.44
1:C:53:LEU:HD22	1:C:225:ILE:CG2	2.47	0.44
1:A:401:THR:HB	1:B:183:GLN:NE2	2.32	0.44
1:C:165:ASN:O	1:C:220:GLU:HB3	2.17	0.44
1:C:350:LEU:HB3	1:C:353:LEU:HD22	1.99	0.44
1:D:350:LEU:HB3	1:D:353:LEU:HD22	1.97	0.44
1:E:337:PRO:O	1:E:366:HIS:HE1	2.00	0.44
1:F:58:LEU:HD13	1:F:60:ARG:HG2	1.98	0.44
1:F:195[A]:LYS:O	1:F:198:PHE:HB2	2.16	0.44
1:F:234:ILE:C	1:F:235:ILE:HD12	2.42	0.44
1:F:344:THR:HG22	1:F:361:GLU:HG3	1.99	0.44
1:B:398:ASN:ND2	1:C:171:LEU:HG	2.31	0.44
1:C:344:THR:HG22	1:C:361:GLU:CG	2.33	0.44
1:A:203:PHE:CE2	1:A:213:LEU:HD21	2.53	0.44
1:A:332:PRO:HG3	1:A:341:ARG:CZ	2.48	0.44
1:C:143:LEU:HD13	1:C:435:PHE:HB2	1.99	0.44
1:D:218:GLU:HG3	1:D:222:LYS:HD2	2.00	0.44
1:F:110:LYS:HE2	1:F:110:LYS:HB2	1.75	0.44
1:F:168:GLN:HE21	1:F:168:GLN:HB3	1.68	0.44
1:F:200:GLU:OE2	1:F:207:ARG:NH1	2.51	0.44
1:F:335:TYR:CE2	1:F:337:PRO:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:O	1:A:105:ARG:HG3	2.18	0.44
1:C:488:ARG:H	1:C:488:ARG:HD2	1.83	0.44
1:D:168:GLN:HE21	1:D:168:GLN:HB3	1.49	0.44
1:B:353:LEU:HD12	1:B:353:LEU:HA	1.84	0.44
1:D:36:PRO:HD2	1:D:173:TYR:CE1	2.53	0.44
1:D:165:ASN:O	1:D:220:GLU:HA	2.18	0.44
1:D:373:PRO:O	1:D:446:LEU:HB2	2.18	0.44
1:D:468:GLN:O	1:D:469:ARG:C	2.61	0.44
1:E:21:ASP:OD1	1:E:35:ASN:HB2	2.18	0.44
1:E:235:ILE:HD13	1:E:235:ILE:N	2.33	0.44
1:A:354:ARG:HG2	1:A:355:TRP:HD1	1.83	0.44
1:B:363:GLY:HA3	1:B:432:TYR:CE1	2.53	0.44
1:A:236:SER:HB2	1:A:237:PRO:CA	2.41	0.43
1:B:189:ASN:HD22	1:B:192:SER:H	1.66	0.43
1:C:141:VAL:HG11	1:C:384:TYR:CE2	2.53	0.43
1:E:190:ILE:HD12	1:F:446:LEU:HD21	1.99	0.43
1:F:55[B]:ARG:HD2	1:F:135:ASP:OD1	2.18	0.43
1:C:334:ILE:HG22	1:C:484:LEU:HD22	2.00	0.43
1:E:128:PHE:CZ	1:E:130:MET:HG3	2.53	0.43
1:A:83:PHE:CE2	1:A:322:LEU:HD21	2.53	0.43
1:C:47:ALA:HA	4:C:507:HOH:O	2.18	0.43
1:D:401:THR:HG21	1:D:404:ASP:HB2	2.01	0.43
1:D:489:GLU:CD	1:D:489:GLU:C	2.85	0.43
1:D:67:PRO:CB	1:D:356:LEU:HD13	2.49	0.43
1:D:195:LYS:HG2	2:D:497:SO4:O1	2.18	0.43
1:F:189:ASN:HD22	1:F:191:PHE:N	2.16	0.43
1:F:214:GLN:HE21	1:F:216:ARG:HE	1.64	0.43
1:B:328:PRO:CG	3:B:504:GOL:H11	2.42	0.43
1:C:320:ALA:HA	3:C:499:GOL:C1	2.49	0.43
1:D:389:ARG:HE	3:D:499:GOL:H12	1.84	0.43
1:D:455:ASN:ND2	1:F:109:GLN:HG3	2.15	0.43
1:E:9:GLU:H	1:E:9:GLU:HG3	1.45	0.43
1:A:370:MET:HG3	1:A:485:VAL:CG1	2.49	0.43
1:C:53:LEU:HD11	1:C:130:MET:HE2	2.01	0.43
1:D:445:ARG:CZ	1:D:482:LYS:HE3	2.49	0.43
1:E:52:THR:C	1:E:53:LEU:HD23	2.42	0.43
1:E:168:GLN:HE21	1:E:168:GLN:HB3	1.43	0.43
1:A:324:LEU:HD22	1:A:345:VAL:CG2	2.49	0.43
1:B:68:GLN:HE21	1:B:159:ARG:HH21	1.66	0.43
1:F:365:LEU:HD13	1:F:370:MET:HA	2.00	0.43
1:A:8:ASN:ND2	1:A:11:GLN:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLN:HB3	3:B:507:GOL:H11	2.01	0.43
1:B:389:ARG:HG2	1:B:408:GLU:CB	2.49	0.43
1:A:449:THR:HB	1:A:482:LYS:HA	2.01	0.43
1:A:450:SER:N	4:A:529:HOH:O	2.42	0.43
1:B:59:ARG:HH21	3:B:506:GOL:C3	2.32	0.43
1:B:328:PRO:HA	3:B:504:GOL:O1	2.19	0.43
1:C:190:ILE:HD12	1:C:191:PHE:H	1.84	0.43
1:D:345:VAL:O	1:D:359:SER:HB2	2.18	0.43
1:D:381:SER:HB2	1:D:415:VAL:HB	2.01	0.43
1:F:145:ASP:HB2	1:F:358:LEU:HD11	2.00	0.43
1:F:189:ASN:ND2	1:F:189:ASN:C	2.77	0.43
1:A:196:ARG:HB3	1:A:207:ARG:HH21	1.84	0.42
1:A:200:GLU:OE2	1:A:207:ARG:NH2	2.51	0.42
1:A:354:ARG:HG2	1:A:355:TRP:CD1	2.54	0.42
1:C:76:ASN:HD22	1:C:115:ARG:HB3	1.84	0.42
1:E:171:LEU:HG	1:F:398:ASN:ND2	2.34	0.42
1:F:196:ARG:HD2	1:F:207:ARG:NH1	2.34	0.42
1:F:370:MET:HG3	1:F:485:VAL:CG1	2.47	0.42
1:A:35:ASN:HA	1:A:36:PRO:HD2	1.84	0.42
1:A:417:GLN:O	1:A:418:ASN:HB2	2.18	0.42
1:C:20:PRO:HG3	1:C:34:TRP:CZ2	2.53	0.42
1:D:169:GLU:H	1:D:169:GLU:CD	2.21	0.42
1:F:81:MET:HA	1:F:127:VAL:O	2.19	0.42
1:A:82:VAL:HG11	1:C:452:VAL:HA	2.00	0.42
1:A:111:VAL:HG21	1:A:234:ILE:HG21	2.01	0.42
1:A:113:ARG:NH2	4:A:543:HOH:O	2.52	0.42
1:B:15:LEU:HB2	1:B:403:PHE:HB2	2.01	0.42
1:E:109:GLN:HG3	1:F:455:ASN:ND2	2.33	0.42
1:E:162:LEU:CD2	1:E:190:ILE:HD11	2.49	0.42
1:A:401:THR:HB	1:B:183:GLN:HE21	1.84	0.42
1:D:336:ASN:HA	1:D:337:PRO:HD2	1.89	0.42
1:B:432:TYR:CD2	1:B:432:TYR:C	2.98	0.42
1:B:437:THR:OG1	1:C:152:GLN:NE2	2.48	0.42
1:D:328:PRO:CG	3:D:500:GOL:H31	2.30	0.42
1:F:146:ILE:CD1	1:F:157:PRO:HD3	2.50	0.42
1:F:334:ILE:O	1:F:341:ARG:HA	2.20	0.42
1:B:341:ARG:O	1:B:342:ILE:HD13	2.19	0.42
1:C:394:VAL:HA	1:C:420:ALA:O	2.20	0.42
1:D:52:THR:HA	1:D:138:VAL:O	2.19	0.42
1:A:105:ARG:N	1:A:106:ASP:CA	2.80	0.42
1:A:383:ILE:O	1:A:412:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:LEU:CD1	1:C:444:ALA:HB2	2.49	0.42
1:D:189:ASN:HD22	1:D:191:PHE:H	1.68	0.42
1:D:351:PRO:O	1:D:354:ARG:HG2	2.20	0.42
1:E:200:GLU:O	1:E:204:ASN:N	2.51	0.42
1:E:330:SER:OG	1:E:343:LYS:HG3	2.20	0.42
1:F:485:VAL:HA	1:F:486:PRO:HD3	1.84	0.42
1:B:38:ASN:O	1:B:39:LYS:C	2.61	0.42
1:C:234:ILE:HG22	1:C:235:ILE:N	2.33	0.42
1:D:81:MET:HE2	1:D:122:VAL:HG22	2.02	0.42
1:E:219:ASP:OD2	1:E:220:GLU:N	2.53	0.42
1:F:7:GLN:HG2	1:F:8:ASN:ND2	2.34	0.42
1:F:190:ILE:HD12	1:F:191:PHE:N	2.35	0.42
1:B:53:LEU:HD22	1:B:225:ILE:CG2	2.49	0.42
1:B:90:PHE:CB	1:B:106:ASP:O	2.68	0.42
1:B:220:GLU:O	1:B:220:GLU:HG3	2.19	0.42
1:C:145:ASP:OD1	1:C:147:ARG:HG2	2.20	0.42
1:C:157:PRO:HB2	1:C:170:PHE:CD2	2.54	0.42
1:C:189:ASN:HD22	1:C:192:SER:H	1.67	0.42
1:A:109:GLN:HG3	1:C:455:ASN:ND2	2.34	0.42
1:C:357:LYS:HD3	1:C:439:ASP:OD1	2.20	0.42
1:F:214:GLN:HE22	1:F:216:ARG:HE	1.65	0.42
1:A:353:LEU:HG	1:A:358:LEU:O	2.19	0.41
1:B:66:ALA:HB1	1:B:67:PRO:HD2	2.01	0.41
1:B:465:PHE:CE1	1:C:163:ALA:HB2	2.56	0.41
1:C:152:GLN:HE21	1:C:152:GLN:HB3	1.62	0.41
1:E:90:PHE:HD2	1:E:108:HIS:CE1	2.38	0.41
1:A:105:ARG:O	1:A:105:ARG:CG	2.67	0.41
1:C:196:ARG:HG2	1:C:214:GLN:HE22	1.84	0.41
1:C:336:ASN:HA	1:C:337:PRO:HD3	1.79	0.41
1:D:156:MET:HE1	1:D:173:TYR:HB2	2.02	0.41
1:D:219:ASP:OD1	1:D:219:ASP:N	2.48	0.41
1:E:143:LEU:HD13	1:E:435:PHE:HB3	2.02	0.41
1:E:146:ILE:HD13	1:E:155:GLN:O	2.19	0.41
1:F:408:GLU:HG2	4:F:509:HOH:O	2.20	0.41
1:D:143:LEU:HD13	1:D:435:PHE:CB	2.50	0.41
1:E:394:VAL:HA	1:E:420:ALA:O	2.21	0.41
1:F:115:ARG:NH1	3:F:498:GOL:O2	2.53	0.41
1:A:80:GLY:O	1:A:128:PHE:HA	2.21	0.41
1:B:317:VAL:CG1	1:B:319:THR:HG22	2.50	0.41
1:D:485:VAL:HA	1:D:486:PRO:HD3	1.95	0.41
1:E:86:CYS:HB2	1:E:109:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:VAL:HG11	1:E:384:TYR:CE2	2.55	0.41
1:E:330:SER:HB2	1:E:343:LYS:HE2	2.02	0.41
1:A:8:ASN:HD22	1:A:11:GLN:HB2	1.85	0.41
1:A:171:LEU:HD23	1:C:398:ASN:ND2	2.36	0.41
1:B:47:ALA:HB2	1:B:157:PRO:HG3	2.03	0.41
1:B:331:SER:HA	1:B:332:PRO:HD3	1.84	0.41
1:B:427:SER:CB	3:B:505:GOL:H32	2.50	0.41
1:C:160:PHE:CD1	1:C:160:PHE:N	2.88	0.41
1:D:110:LYS:O	1:D:110:LYS:HG3	2.20	0.41
1:E:168:GLN:HG2	1:E:169:GLU:N	2.34	0.41
1:E:401:THR:HG21	1:E:404:ASP:HB2	2.02	0.41
1:F:366:HIS:O	1:F:425:SER:HB3	2.21	0.41
1:A:350:LEU:O	1:A:353:LEU:HB2	2.21	0.41
1:C:235:ILE:O	1:C:235:ILE:HG22	2.20	0.41
1:C:316:THR:HG22	1:C:355:TRP:HZ2	1.85	0.41
1:D:186:GLU:CG	1:D:187:GLY:H	2.34	0.41
1:E:52:THR:HA	1:E:138:VAL:O	2.20	0.41
1:E:147:ARG:O	1:E:148:SER:C	2.63	0.41
1:A:408:GLU:O	1:A:409:ALA:C	2.61	0.41
1:E:146:ILE:HD11	1:E:157:PRO:HD3	2.03	0.41
1:E:160:PHE:CE2	1:F:397:CYS:HB3	2.55	0.41
1:E:202:ALA:O	1:F:479:ASN:ND2	2.52	0.41
1:F:377:LEU:HD11	1:F:444:ALA:HB2	2.01	0.41
1:B:83:PHE:HA	1:B:84:PRO:HD2	1.83	0.41
1:B:475:LEU:HD21	1:C:213:LEU:HD13	2.02	0.41
1:C:143:LEU:HD13	1:C:435:PHE:CB	2.51	0.41
1:D:115:ARG:HH12	3:D:498:GOL:H31	1.86	0.41
1:D:196:ARG:HG2	1:D:207:ARG:NE	2.36	0.41
1:E:76:ASN:ND2	1:E:116:GLU:H	2.19	0.41
1:B:90:PHE:HB2	1:B:106:ASP:O	2.21	0.41
1:C:205:VAL:HB	1:C:209:ILE:HD12	2.02	0.41
1:C:374:HIS:CE1	3:C:500:GOL:H2	2.56	0.41
1:D:446:LEU:HD12	1:D:446:LEU:HA	1.87	0.41
1:D:465:PHE:CE1	1:F:163:ALA:HB2	2.56	0.41
1:E:56:ASN:HA	1:E:132:ASN:O	2.21	0.41
1:E:69:GLU:HB2	1:E:358:LEU:HD13	2.02	0.41
1:F:391:ARG:NH1	1:F:404:ASP:OD1	2.53	0.41
1:A:109:GLN:HG3	1:C:455:ASN:HD22	1.86	0.41
1:C:88:GLU:HB3	1:C:89:THR:H	1.72	0.41
1:C:394:VAL:O	1:C:402:VAL:HG22	2.21	0.41
1:D:394:VAL:HG13	1:D:403:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:SER:HB2	1:E:222:LYS:O	2.21	0.41
1:F:417:GLN:O	1:F:418:ASN:HB2	2.21	0.41
1:B:346:THR:HB	1:B:439:ASP:O	2.20	0.40
1:C:371:PHE:CD1	1:C:371:PHE:C	2.99	0.40
1:D:168:GLN:HE22	1:E:398:ASN:HD21	1.69	0.40
1:D:201:ASP:OD1	1:E:488:ARG:HD3	2.20	0.40
1:E:171:LEU:HG	1:F:398:ASN:HD21	1.86	0.40
1:F:146:ILE:HD13	1:F:157:PRO:HD3	2.03	0.40
1:D:196:ARG:NH2	1:D:216:ARG:HH11	2.20	0.40
1:A:474:GLN:HE21	1:A:478:ASN:ND2	2.19	0.40
1:D:196:ARG:HD2	1:D:211:ASP:OD1	2.20	0.40
1:E:113:ARG:NH2	1:E:133:ASP:OD2	2.54	0.40
1:A:452:VAL:HA	1:B:82:VAL:HG11	2.02	0.40
1:C:68:GLN:HB2	1:C:122:VAL:HB	2.03	0.40
1:C:485:VAL:HA	1:C:486:PRO:HD3	1.79	0.40
1:F:320:ALA:O	1:F:322:LEU:HD22	2.22	0.40
1:A:212:ARG:HG3	1:C:467:LEU:HD23	2.02	0.40
1:A:236:SER:CB	1:A:237:PRO:HA	2.40	0.40
1:A:331:SER:HA	1:A:332:PRO:HD3	1.85	0.40
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.94	0.40
1:B:389:ARG:HD3	3:B:505:GOL:C1	2.41	0.40
1:C:350:LEU:O	1:C:353:LEU:HB2	2.22	0.40
1:C:367:LYS:HB2	1:C:428:ASP:HA	2.02	0.40
1:C:457:PRO:O	1:C:461:VAL:HG23	2.22	0.40
1:D:53:LEU:HD22	1:D:225:ILE:HD13	2.04	0.40
1:D:189:ASN:HD21	1:D:191:PHE:HB2	1.87	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	372/496 (75%)	350 (94%)	20 (5%)	2 (0%)	24	46
1	B	375/496 (76%)	356 (95%)	18 (5%)	1 (0%)	36	58
1	C	367/496 (74%)	341 (93%)	26 (7%)	0	100	100
1	D	368/496 (74%)	344 (94%)	24 (6%)	0	100	100
1	E	375/496 (76%)	353 (94%)	21 (6%)	1 (0%)	36	58
1	F	371/496 (75%)	353 (95%)	17 (5%)	1 (0%)	36	58
All	All	2228/2976 (75%)	2097 (94%)	126 (6%)	5 (0%)	43	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	236	SER
1	F	87	PRO
1	A	153	LEU
1	B	153	LEU
1	A	235	ILE

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	324/425 (76%)	294 (91%)	30 (9%)	8	18
1	B	327/425 (77%)	297 (91%)	30 (9%)	8	19
1	C	319/425 (75%)	285 (89%)	34 (11%)	6	14
1	D	320/425 (75%)	290 (91%)	30 (9%)	8	18
1	E	327/425 (77%)	294 (90%)	33 (10%)	7	15
1	F	323/425 (76%)	281 (87%)	42 (13%)	4	8
All	All	1940/2550 (76%)	1741 (90%)	199 (10%)	7	15

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	21	ASP
1	A	48	LEU
1	A	53	LEU
1	A	58	LEU
1	A	111	VAL
1	A	141	VAL
1	A	143	LEU
1	A	155	GLN
1	A	168	GLN
1	A	171	LEU
1	A	189	ASN
1	A	190	ILE
1	A	199	LEU
1	A	221	GLU
1	A	226	VAL
1	A	322	LEU
1	A	323	ARG
1	A	353	LEU
1	A	391	ARG
1	A	394	VAL
1	A	395	VAL
1	A	446	LEU
1	A	449	THR
1	A	454	ASN
1	A	460	VAL
1	A	470	ASN
1	A	484	LEU
1	A	485	VAL
1	A	488	ARG
1	B	9	GLU
1	B	14	ARG
1	B	48	LEU
1	B	58	LEU
1	B	86	CYS
1	B	111	VAL
1	B	135	ASP
1	B	141	VAL
1	B	147	ARG
1	B	168	GLN
1	B	171	LEU
1	B	175	HIS
1	B	184	GLU

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Mol	Chain	Res	Type
1	B	186	GLU
1	B	189	ASN
1	B	199	LEU
1	B	232	LEU
1	B	234	ILE
1	B	235	ILE
1	B	322	LEU
1	B	324	LEU
1	B	353	LEU
1	B	394	VAL
1	B	395	VAL
1	B	446	LEU
1	B	459	ASP
1	B	460	VAL
1	B	484	LEU
1	B	485	VAL
1	B	488	ARG
1	C	22	ASN
1	C	23	ARG
1	C	48	LEU
1	C	58	LEU
1	C	110	LYS
1	C	111	VAL
1	C	115	ARG
1	C	135	ASP
1	C	141	VAL
1	C	168	GLN
1	C	171	LEU
1	C	172	GLN
1	C	189	ASN
1	C	190	ILE
1	C	199	LEU
1	C	220	GLU
1	C	226	VAL
1	C	317	VAL
1	C	318	CYS
1	C	322	LEU
1	C	323	ARG
1	C	353	LEU
1	C	356	LEU
1	C	391	ARG
1	C	394	VAL

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Mol	Chain	Res	Type
1	C	395	VAL
1	C	429	ARG
1	C	443	ILE
1	C	446	LEU
1	C	449	THR
1	C	460	VAL
1	C	484	LEU
1	C	485	VAL
1	C	488	ARG
1	D	14	ARG
1	D	23	ARG
1	D	26	SER
1	D	48	LEU
1	D	53	LEU
1	D	58	LEU
1	D	88	GLU
1	D	107	ARG
1	D	111	VAL
1	D	113	ARG
1	D	141	VAL
1	D	142	SER
1	D	152	GLN
1	D	168	GLN
1	D	171	LEU
1	D	172	GLN
1	D	196	ARG
1	D	199	LEU
1	D	229	LYS
1	D	322	LEU
1	D	353	LEU
1	D	356	LEU
1	D	391	ARG
1	D	394	VAL
1	D	395	VAL
1	D	446	LEU
1	D	449	THR
1	D	460	VAL
1	D	484	LEU
1	D	485	VAL
1	E	9	GLU
1	E	22	ASN
1	E	48	LEU

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Mol	Chain	Res	Type
1	E	58	LEU
1	E	89	THR
1	E	103	ARG
1	E	107	ARG
1	E	110	LYS
1	E	111	VAL
1	E	113	ARG
1	E	135	ASP
1	E	141	VAL
1	E	168	GLN
1	E	171	LEU
1	E	199	LEU
1	E	226	VAL
1	E	229	LYS
1	E	234	ILE
1	E	235	ILE
1	E	317	VAL
1	E	322	LEU
1	E	329	SER
1	E	331	SER
1	E	353	LEU
1	E	391	ARG
1	E	394	VAL
1	E	395	VAL
1	E	443	ILE
1	E	446	LEU
1	E	454	ASN
1	E	460	VAL
1	E	484	LEU
1	E	485	VAL
1	F	9	GLU
1	F	27	GLU
1	F	48	LEU
1	F	53	LEU
1	F	58	LEU
1	F	106	ASP
1	F	110	LYS
1	F	111	VAL
1	F	141	VAL
1	F	147	ARG
1	F	168	GLN
1	F	172	GLN

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Mol	Chain	Res	Type
1	F	175	HIS
1	F	176	GLN
1	F	189	ASN
1	F	190	ILE
1	F	192	SER
1	F	195[A]	LYS
1	F	195[B]	LYS
1	F	199	LEU
1	F	213	LEU
1	F	221	GLU
1	F	226	VAL
1	F	317	VAL
1	F	322	LEU
1	F	344	THR
1	F	353	LEU
1	F	354	ARG
1	F	356	LEU
1	F	387	LYS
1	F	392	LEU
1	F	394	VAL
1	F	395	VAL
1	F	414	THR
1	F	443	ILE
1	F	446	LEU
1	F	449	THR
1	F	453	ILE
1	F	460	VAL
1	F	484	LEU
1	F	485	VAL
1	F	488	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	22	ASN
1	A	37	ASN
1	A	68	GLN
1	A	108	HIS
1	A	152	GLN
1	A	155	GLN
1	A	168	GLN

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Mol	Chain	Res	Type
1	A	172	GLN
1	A	174	GLN
1	A	188	ASN
1	A	189	ASN
1	A	214	GLN
1	A	217	ASN
1	A	366	HIS
1	A	368	ASN
1	A	374	HIS
1	A	398	ASN
1	A	400	ASN
1	A	418	ASN
1	A	455	ASN
1	A	474	GLN
1	B	37	ASN
1	B	38	ASN
1	B	56	ASN
1	B	68	GLN
1	B	76	ASN
1	B	108	HIS
1	B	134	GLN
1	B	152	GLN
1	B	172	GLN
1	B	189	ASN
1	B	208	HIS
1	B	214	GLN
1	B	362	HIS
1	B	368	ASN
1	B	393	GLN
1	B	400	ASN
1	B	418	ASN
1	B	455	ASN
1	B	468	GLN
1	B	470	ASN
1	B	474	GLN
1	C	8	ASN
1	C	56	ASN
1	C	68	GLN
1	C	73	GLN
1	C	76	ASN
1	C	108	HIS
1	C	152	GLN

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Mol	Chain	Res	Type
1	C	172	GLN
1	C	174	GLN
1	C	189	ASN
1	C	214	GLN
1	C	366	HIS
1	C	368	ASN
1	C	400	ASN
1	C	454	ASN
1	C	455	ASN
1	C	470	ASN
1	C	474	GLN
1	D	8	ASN
1	D	37	ASN
1	D	40	GLN
1	D	56	ASN
1	D	76	ASN
1	D	108	HIS
1	D	152	GLN
1	D	155	GLN
1	D	168	GLN
1	D	174	GLN
1	D	189	ASN
1	D	214	GLN
1	D	393	GLN
1	D	400	ASN
1	D	418	ASN
1	D	454	ASN
1	D	455	ASN
1	E	37	ASN
1	E	40	GLN
1	E	56	ASN
1	E	68	GLN
1	E	76	ASN
1	E	108	HIS
1	E	112	ASN
1	E	152	GLN
1	E	172	GLN
1	E	174	GLN
1	E	176	GLN
1	E	188	ASN
1	E	189	ASN
1	E	208	HIS

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Mol	Chain	Res	Type
1	E	214	GLN
1	E	217	ASN
1	E	366	HIS
1	E	368	ASN
1	E	400	ASN
1	E	455	ASN
1	E	468	GLN
1	E	470	ASN
1	F	7	GLN
1	F	8	ASN
1	F	22	ASN
1	F	56	ASN
1	F	68	GLN
1	F	73	GLN
1	F	108	HIS
1	F	152	GLN
1	F	155	GLN
1	F	172	GLN
1	F	174	GLN
1	F	175	HIS
1	F	176	GLN
1	F	189	ASN
1	F	208	HIS
1	F	214	GLN
1	F	217	ASN
1	F	368	ASN
1	F	393	GLN
1	F	398	ASN
1	F	400	ASN
1	F	455	ASN
1	F	468	GLN
1	F	474	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

31 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	499	-	4,4,4	0.26	0	6,6,6	0.17	0
3	GOL	D	498	-	5,5,5	0.37	0	5,5,5	0.29	0
3	GOL	C	500	-	5,5,5	0.45	0	5,5,5	0.66	0
2	SO4	B	498	-	4,4,4	0.29	0	6,6,6	0.15	0
2	SO4	E	498	-	4,4,4	0.26	0	6,6,6	0.11	0
3	GOL	B	503	-	5,5,5	0.30	0	5,5,5	0.41	0
3	GOL	A	500	-	5,5,5	0.33	0	5,5,5	0.29	0
2	SO4	B	501	-	4,4,4	0.25	0	6,6,6	0.11	0
3	GOL	C	502	-	5,5,5	0.41	0	5,5,5	0.46	0
3	GOL	B	505	-	5,5,5	0.37	0	5,5,5	0.52	0
3	GOL	D	499	-	5,5,5	0.38	0	5,5,5	0.27	0
3	GOL	F	497	-	5,5,5	0.31	0	5,5,5	0.50	0
3	GOL	D	500	-	5,5,5	0.38	0	5,5,5	0.30	0
3	GOL	B	504	-	5,5,5	0.40	0	5,5,5	0.63	0
2	SO4	A	498	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	A	497	-	4,4,4	0.28	0	6,6,6	0.06	0
2	SO4	B	500	-	4,4,4	0.22	0	6,6,6	0.12	0
3	GOL	C	499	-	5,5,5	0.37	0	5,5,5	0.40	0
3	GOL	E	499	-	5,5,5	0.36	0	5,5,5	0.34	0
3	GOL	B	507	-	5,5,5	0.40	0	5,5,5	0.39	0
2	SO4	B	497	-	4,4,4	0.26	0	6,6,6	0.22	0
2	SO4	B	502	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	C	497	-	4,4,4	0.24	0	6,6,6	0.13	0
3	GOL	A	499	-	5,5,5	0.40	0	5,5,5	0.22	0
2	SO4	C	498	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	D	497	-	4,4,4	0.24	0	6,6,6	0.13	0
3	GOL	C	501	-	5,5,5	0.35	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	F	498	-	5,5,5	0.40	0	5,5,5	0.36	0
2	SO4	E	497	-	4,4,4	0.26	0	6,6,6	0.10	0
3	GOL	F	499	-	5,5,5	0.36	0	5,5,5	0.23	0
3	GOL	B	506	-	5,5,5	0.45	0	5,5,5	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	504	-	-	4/4/4/4	-
3	GOL	B	507	-	-	2/4/4/4	-
3	GOL	C	500	-	-	1/4/4/4	-
3	GOL	E	499	-	-	2/4/4/4	-
3	GOL	B	503	-	-	4/4/4/4	-
3	GOL	A	500	-	-	0/4/4/4	-
3	GOL	C	502	-	-	4/4/4/4	-
3	GOL	B	505	-	-	2/4/4/4	-
3	GOL	D	499	-	-	2/4/4/4	-
3	GOL	D	498	-	-	0/4/4/4	-
3	GOL	A	499	-	-	3/4/4/4	-
3	GOL	C	501	-	-	0/4/4/4	-
3	GOL	F	498	-	-	4/4/4/4	-
3	GOL	C	499	-	-	2/4/4/4	-
3	GOL	F	497	-	-	2/4/4/4	-
3	GOL	F	499	-	-	2/4/4/4	-
3	GOL	D	500	-	-	4/4/4/4	-
3	GOL	B	506	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	GOL	O1-C1-C2-C3
3	B	503	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	504	GOL	O1-C1-C2-C3
3	B	505	GOL	O1-C1-C2-C3
3	B	506	GOL	C1-C2-C3-O3
3	B	507	GOL	O1-C1-C2-O2
3	B	507	GOL	O1-C1-C2-C3
3	C	499	GOL	O1-C1-C2-C3
3	D	499	GOL	O1-C1-C2-C3
3	D	500	GOL	O1-C1-C2-C3
3	E	499	GOL	O1-C1-C2-C3
3	F	498	GOL	O1-C1-C2-C3
3	F	498	GOL	C1-C2-C3-O3
3	F	499	GOL	O1-C1-C2-C3
3	F	498	GOL	O1-C1-C2-O2
3	A	499	GOL	C1-C2-C3-O3
3	B	504	GOL	C1-C2-C3-O3
3	B	506	GOL	O1-C1-C2-C3
3	C	502	GOL	O1-C1-C2-C3
3	C	502	GOL	C1-C2-C3-O3
3	D	500	GOL	C1-C2-C3-O3
3	F	497	GOL	O1-C1-C2-C3
3	B	503	GOL	O1-C1-C2-O2
3	B	503	GOL	O2-C2-C3-O3
3	B	504	GOL	O1-C1-C2-O2
3	B	505	GOL	O1-C1-C2-O2
3	B	506	GOL	O1-C1-C2-O2
3	B	506	GOL	O2-C2-C3-O3
3	C	502	GOL	O1-C1-C2-O2
3	D	500	GOL	O1-C1-C2-O2
3	F	497	GOL	O1-C1-C2-O2
3	A	499	GOL	O2-C2-C3-O3
3	C	499	GOL	O1-C1-C2-O2
3	D	499	GOL	O1-C1-C2-O2
3	E	499	GOL	O1-C1-C2-O2
3	F	498	GOL	O2-C2-C3-O3
3	A	499	GOL	O1-C1-C2-O2
3	D	500	GOL	O2-C2-C3-O3
3	F	499	GOL	O1-C1-C2-O2
3	B	504	GOL	O2-C2-C3-O3
3	C	502	GOL	O2-C2-C3-O3
3	C	500	GOL	O2-C2-C3-O3

There are no ring outliers.

17 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	498	GOL	1	0
3	C	500	GOL	3	0
3	B	503	GOL	6	0
3	A	500	GOL	2	0
3	C	502	GOL	3	0
3	B	505	GOL	4	0
3	D	499	GOL	5	0
3	F	497	GOL	1	0
3	D	500	GOL	2	0
3	B	504	GOL	10	0
3	C	499	GOL	4	0
3	B	507	GOL	3	0
2	D	497	SO4	1	0
3	C	501	GOL	1	0
3	F	498	GOL	2	0
3	F	499	GOL	4	0
3	B	506	GOL	4	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	380/496 (76%)	-1.69	0 100 100	20, 34, 69, 124	0
1	B	383/496 (77%)	-1.74	0 100 100	18, 31, 66, 106	0
1	C	375/496 (75%)	-1.71	0 100 100	20, 32, 60, 96	0
1	D	376/496 (75%)	-1.75	0 100 100	18, 31, 60, 105	0
1	E	383/496 (77%)	-1.70	0 100 100	18, 32, 62, 113	0
1	F	377/496 (76%)	-1.67	0 100 100	20, 36, 68, 103	2 (0%)
All	All	2274/2976 (76%)	-1.71	0 100 100	18, 33, 65, 124	2 (0%)

There are no RSRZ outliers to report.

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
3	GOL	A	499	6/6	0.98	0.05	30,55,58,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	500	6/6	0.98	0.07	46,52,52,53	0
3	GOL	F	497	6/6	0.98	0.04	43,56,59,61	0
3	GOL	F	498	6/6	0.98	0.07	44,55,58,59	0
3	GOL	F	499	6/6	0.98	0.05	57,61,70,71	0
2	SO4	C	498	5/5	0.99	0.05	52,55,67,68	0
2	SO4	D	497	5/5	0.99	0.03	59,66,79,81	0
2	SO4	E	497	5/5	0.99	0.06	59,69,83,92	0
2	SO4	E	498	5/5	0.99	0.04	67,74,89,95	0
2	SO4	A	497	5/5	0.99	0.04	46,50,66,74	0
3	GOL	A	500	6/6	0.99	0.04	45,51,57,60	0
3	GOL	B	504	6/6	0.99	0.06	37,38,41,43	0
3	GOL	B	505	6/6	0.99	0.04	31,42,42,64	0
3	GOL	B	507	6/6	0.99	0.04	35,43,51,59	0
3	GOL	C	499	6/6	0.99	0.04	37,54,64,64	0
3	GOL	C	501	6/6	0.99	0.04	44,49,51,52	0
3	GOL	C	502	6/6	0.99	0.06	43,45,52,56	0
3	GOL	D	498	6/6	0.99	0.03	42,51,57,59	0
3	GOL	D	499	6/6	0.99	0.03	41,45,50,56	0
2	SO4	A	498	5/5	0.99	0.04	64,66,74,78	0
3	GOL	E	499	6/6	0.99	0.05	30,43,48,57	0
2	SO4	B	500	5/5	0.99	0.02	46,56,68,70	0
2	SO4	B	502	5/5	0.99	0.03	63,70,84,86	0
2	SO4	C	497	5/5	0.99	0.04	56,58,68,80	0
2	SO4	B	499	5/5	1.00	0.01	41,43,48,52	0
3	GOL	B	506	6/6	1.00	0.04	13,28,31,34	0
2	SO4	B	497	5/5	1.00	0.01	40,42,49,55	0
2	SO4	B	501	5/5	1.00	0.03	46,52,66,66	0
3	GOL	C	500	6/6	1.00	0.03	34,37,39,44	0
3	GOL	B	503	6/6	1.00	0.03	37,43,47,48	0
2	SO4	B	498	5/5	1.00	0.04	28,29,33,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.