



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:06 am GMT

PDB ID : 4BSS
Title : Structure of the ectodomain of LGR5 in complex with R-spondin-1 (Fu1Fu2) in P21 crystal form
Authors : Peng, W.C.; de Lau, W.; Forneris, F.; Granneman, J.C.M.; Huch, M.; Clevers, H.; Gros, P.
Deposited on : 2013-06-11
Resolution : 3.20 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

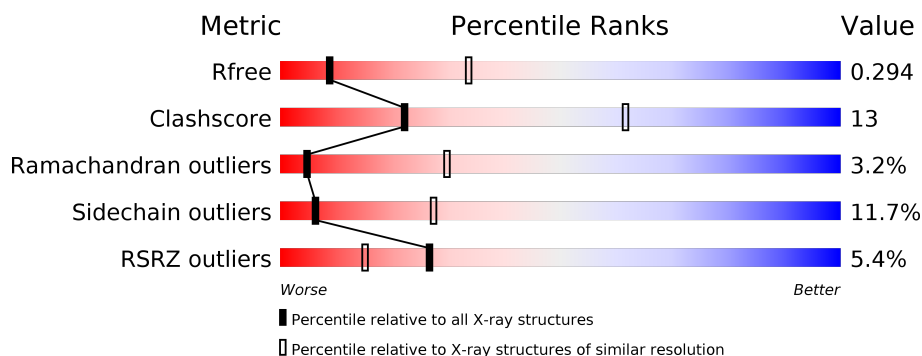
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	539	<div> <div>13%</div> <div>59% 24% 14%</div> </div>
1	B	539	<div> <div>57% 25% 13%</div> </div>
1	E	539	<div> <div>5% 48% 32% 7% 13%</div> </div>
1	F	539	<div> <div>3% 56% 26% 14%</div> </div>
2	C	126	<div> <div>13% 54% 22% 6% 18%</div> </div>
2	D	126	<div> <div>3% 63% 15% 5% 17%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	126	
2	H	126	

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	NAG	A	1208	X	-	-	-
3	NAG	E	1063	-	-	-	X
3	NAG	E	1064	-	-	-	X
4	NAG	F	1077	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17925 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 LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	68	0	0
			3653	2328	627	682	16			
1	B	469	Total	C	N	O	S	42	0	0
			3671	2342	633	679	17			
1	E	468	Total	C	N	O	S	53	0	0
			3672	2339	630	686	17			
1	F	464	Total	C	N	O	S	46	0	0
			3637	2320	626	674	17			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	HIS	-	EXPRESSION TAG	UNP O75473
A	9	HIS	-	EXPRESSION TAG	UNP O75473
A	10	HIS	-	EXPRESSION TAG	UNP O75473
A	11	HIS	-	EXPRESSION TAG	UNP O75473
A	12	HIS	-	EXPRESSION TAG	UNP O75473
A	13	HIS	-	EXPRESSION TAG	UNP O75473
A	14	GLU	-	EXPRESSION TAG	UNP O75473
A	15	ASN	-	EXPRESSION TAG	UNP O75473
A	16	LEU	-	EXPRESSION TAG	UNP O75473
A	17	TYR	-	EXPRESSION TAG	UNP O75473
A	18	PHE	-	EXPRESSION TAG	UNP O75473
A	19	GLN	-	EXPRESSION TAG	UNP O75473
A	20	GLY	-	EXPRESSION TAG	UNP O75473
A	21	SER	-	EXPRESSION TAG	UNP O75473
A	544	ALA	-	EXPRESSION TAG	UNP O75473
A	545	ALA	-	EXPRESSION TAG	UNP O75473
A	546	ALA	-	EXPRESSION TAG	UNP O75473
B	8	HIS	-	EXPRESSION TAG	UNP O75473
B	9	HIS	-	EXPRESSION TAG	UNP O75473
B	10	HIS	-	EXPRESSION TAG	UNP O75473

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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	EXPRESSION TAG	UNP O75473
B	12	HIS	-	EXPRESSION TAG	UNP O75473
B	13	HIS	-	EXPRESSION TAG	UNP O75473
B	14	GLU	-	EXPRESSION TAG	UNP O75473
B	15	ASN	-	EXPRESSION TAG	UNP O75473
B	16	LEU	-	EXPRESSION TAG	UNP O75473
B	17	TYR	-	EXPRESSION TAG	UNP O75473
B	18	PHE	-	EXPRESSION TAG	UNP O75473
B	19	GLN	-	EXPRESSION TAG	UNP O75473
B	20	GLY	-	EXPRESSION TAG	UNP O75473
B	21	SER	-	EXPRESSION TAG	UNP O75473
B	544	ALA	-	EXPRESSION TAG	UNP O75473
B	545	ALA	-	EXPRESSION TAG	UNP O75473
B	546	ALA	-	EXPRESSION TAG	UNP O75473
E	8	HIS	-	EXPRESSION TAG	UNP O75473
E	9	HIS	-	EXPRESSION TAG	UNP O75473
E	10	HIS	-	EXPRESSION TAG	UNP O75473
E	11	HIS	-	EXPRESSION TAG	UNP O75473
E	12	HIS	-	EXPRESSION TAG	UNP O75473
E	13	HIS	-	EXPRESSION TAG	UNP O75473
E	14	GLU	-	EXPRESSION TAG	UNP O75473
E	15	ASN	-	EXPRESSION TAG	UNP O75473
E	16	LEU	-	EXPRESSION TAG	UNP O75473
E	17	TYR	-	EXPRESSION TAG	UNP O75473
E	18	PHE	-	EXPRESSION TAG	UNP O75473
E	19	GLN	-	EXPRESSION TAG	UNP O75473
E	20	GLY	-	EXPRESSION TAG	UNP O75473
E	21	SER	-	EXPRESSION TAG	UNP O75473
E	544	ALA	-	EXPRESSION TAG	UNP O75473
E	545	ALA	-	EXPRESSION TAG	UNP O75473
E	546	ALA	-	EXPRESSION TAG	UNP O75473
F	8	HIS	-	EXPRESSION TAG	UNP O75473
F	9	HIS	-	EXPRESSION TAG	UNP O75473
F	10	HIS	-	EXPRESSION TAG	UNP O75473
F	11	HIS	-	EXPRESSION TAG	UNP O75473
F	12	HIS	-	EXPRESSION TAG	UNP O75473
F	13	HIS	-	EXPRESSION TAG	UNP O75473
F	14	GLU	-	EXPRESSION TAG	UNP O75473
F	15	ASN	-	EXPRESSION TAG	UNP O75473
F	16	LEU	-	EXPRESSION TAG	UNP O75473
F	17	TYR	-	EXPRESSION TAG	UNP O75473
F	18	PHE	-	EXPRESSION TAG	UNP O75473

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Chain	Residue	Modelled	Actual	Comment	Reference
F	19	GLN	-	EXPRESSION TAG	UNP O75473
F	20	GLY	-	EXPRESSION TAG	UNP O75473
F	21	SER	-	EXPRESSION TAG	UNP O75473
F	544	ALA	-	EXPRESSION TAG	UNP O75473
F	545	ALA	-	EXPRESSION TAG	UNP O75473
F	546	ALA	-	EXPRESSION TAG	UNP O75473

- Molecule 2 is a protein called R-SPONDIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	103	Total	C	N	O	S	0	0	0
			778	480	137	143	18			
2	D	104	Total	C	N	O	S	0	0	0
			784	483	138	145	18			
2	G	103	Total	C	N	O	S	0	0	0
			778	480	137	143	18			
2	H	104	Total	C	N	O	S	0	0	0
			784	483	138	145	18			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	GLY	-	EXPRESSION TAG	UNP Q2MKA7
C	30	SER	-	EXPRESSION TAG	UNP Q2MKA7
C	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7
C	148	ALA	-	EXPRESSION TAG	UNP Q2MKA7
C	149	HIS	-	EXPRESSION TAG	UNP Q2MKA7
C	150	HIS	-	EXPRESSION TAG	UNP Q2MKA7
C	151	HIS	-	EXPRESSION TAG	UNP Q2MKA7
C	152	HIS	-	EXPRESSION TAG	UNP Q2MKA7
C	153	HIS	-	EXPRESSION TAG	UNP Q2MKA7
C	154	HIS	-	EXPRESSION TAG	UNP Q2MKA7
D	29	GLY	-	EXPRESSION TAG	UNP Q2MKA7
D	30	SER	-	EXPRESSION TAG	UNP Q2MKA7
D	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7
D	148	ALA	-	EXPRESSION TAG	UNP Q2MKA7
D	149	HIS	-	EXPRESSION TAG	UNP Q2MKA7
D	150	HIS	-	EXPRESSION TAG	UNP Q2MKA7
D	151	HIS	-	EXPRESSION TAG	UNP Q2MKA7
D	152	HIS	-	EXPRESSION TAG	UNP Q2MKA7
D	153	HIS	-	EXPRESSION TAG	UNP Q2MKA7
D	154	HIS	-	EXPRESSION TAG	UNP Q2MKA7

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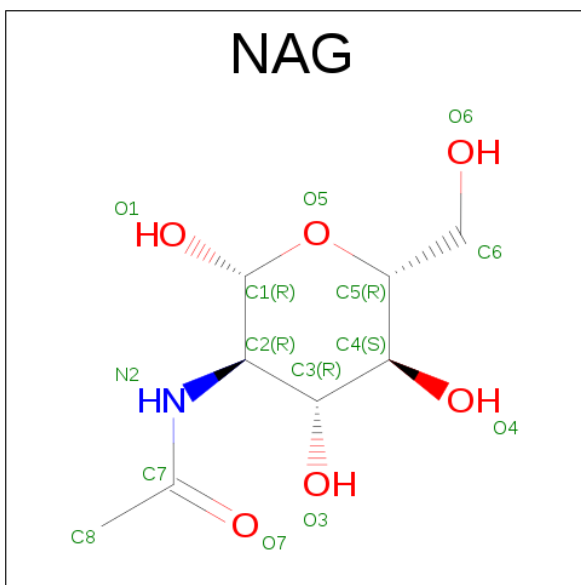
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Chain	Residue	Modelled	Actual	Comment	Reference
G	29	GLY	-	EXPRESSION TAG	UNP Q2MKA7
G	30	SER	-	EXPRESSION TAG	UNP Q2MKA7
G	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7
G	148	ALA	-	EXPRESSION TAG	UNP Q2MKA7
G	149	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	150	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	151	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	152	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	153	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	154	HIS	-	EXPRESSION TAG	UNP Q2MKA7
H	29	GLY	-	EXPRESSION TAG	UNP Q2MKA7
H	30	SER	-	EXPRESSION TAG	UNP Q2MKA7
H	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7
H	148	ALA	-	EXPRESSION TAG	UNP Q2MKA7
H	149	HIS	-	EXPRESSION TAG	UNP Q2MKA7
H	150	HIS	-	EXPRESSION TAG	UNP Q2MKA7
H	151	HIS	-	EXPRESSION TAG	UNP Q2MKA7
H	152	HIS	-	EXPRESSION TAG	UNP Q2MKA7
H	153	HIS	-	EXPRESSION TAG	UNP Q2MKA7
H	154	HIS	-	EXPRESSION TAG	UNP Q2MKA7

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).

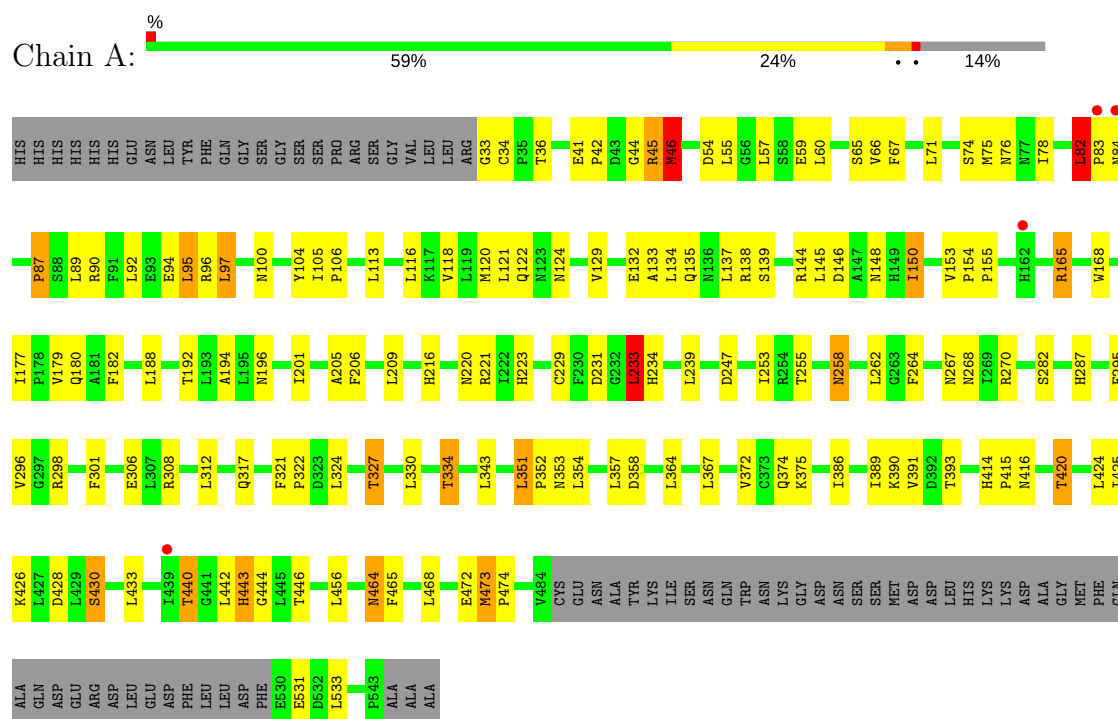


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

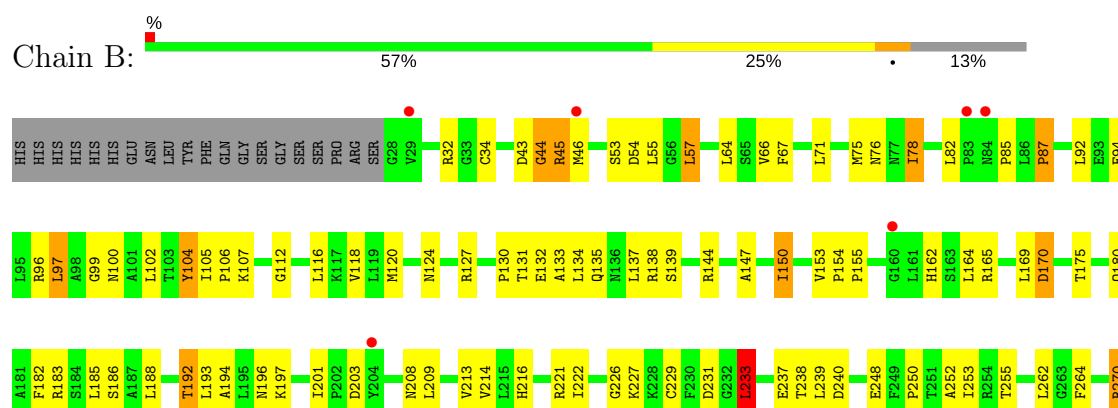
3 Residue-property plots

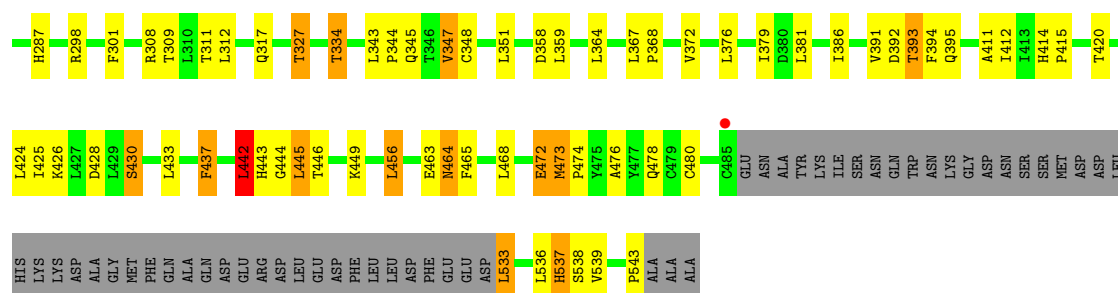
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR



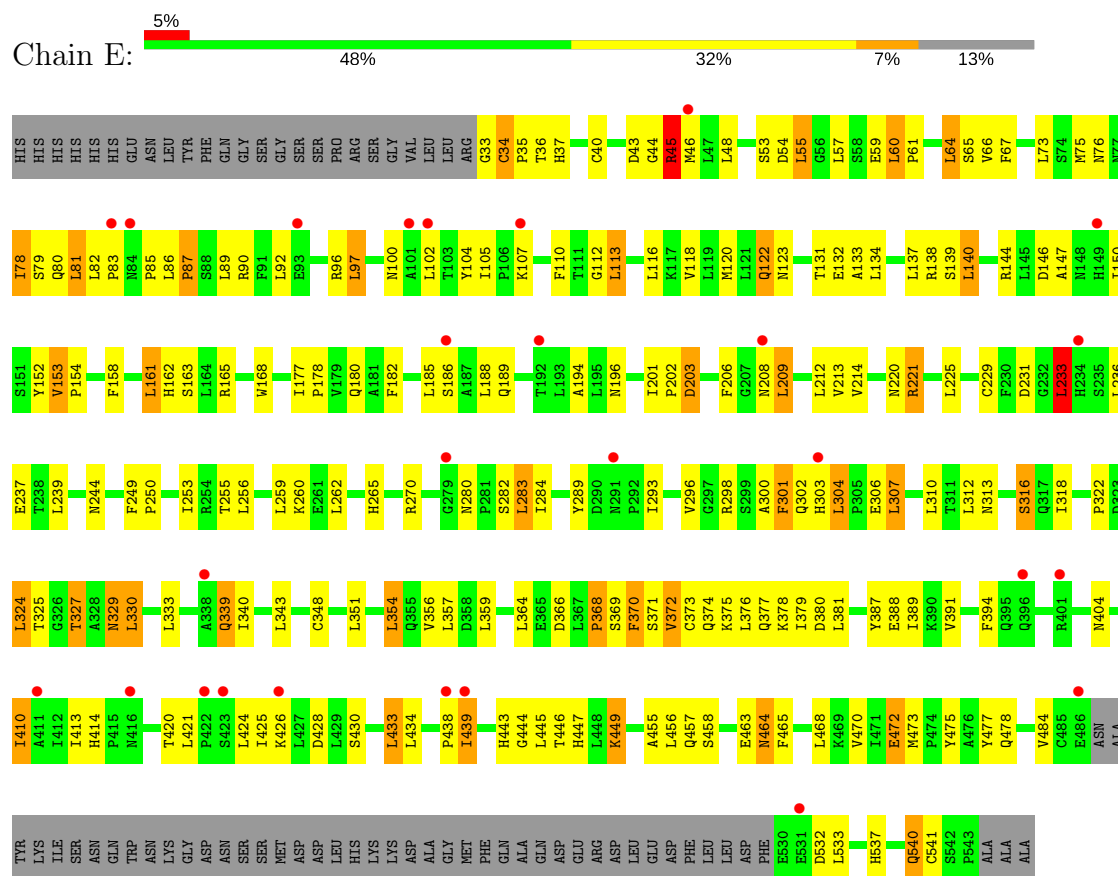
- Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR





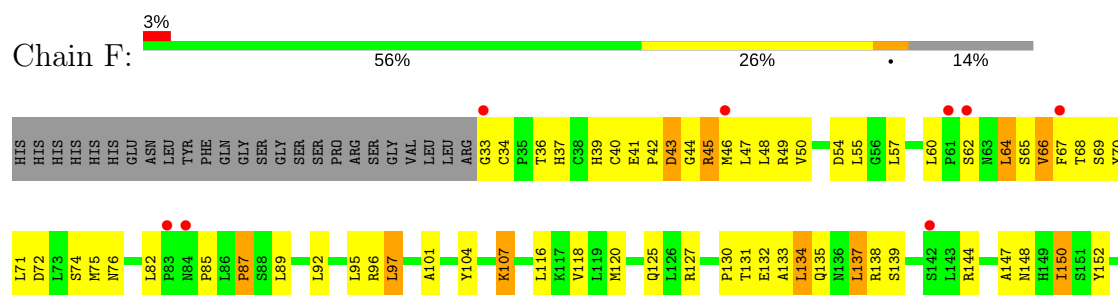
• Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR

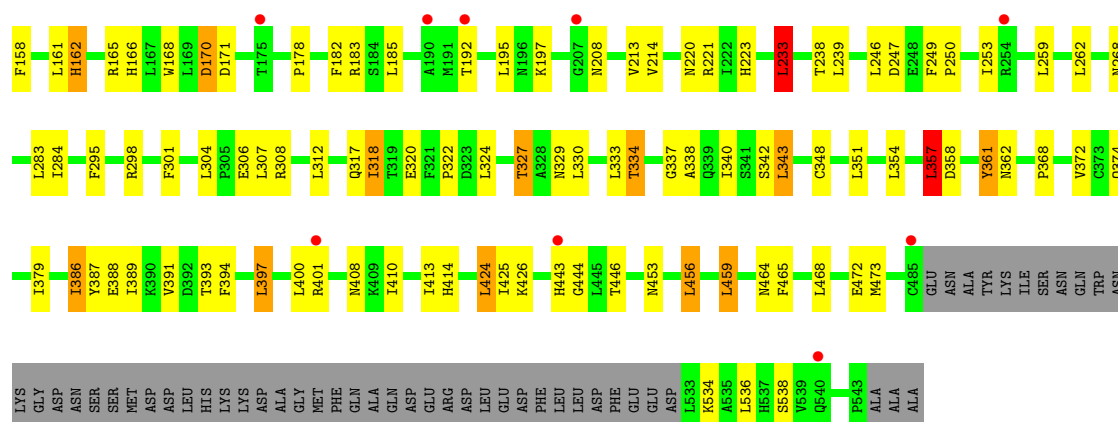
5



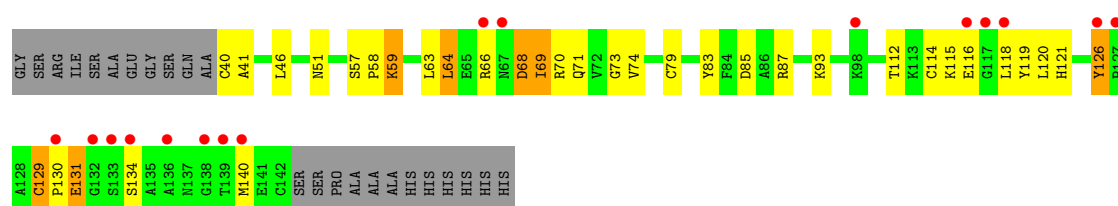
• Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR

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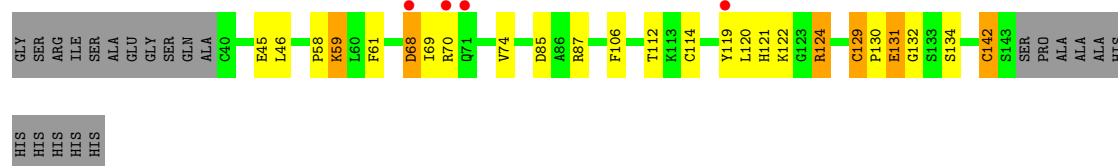




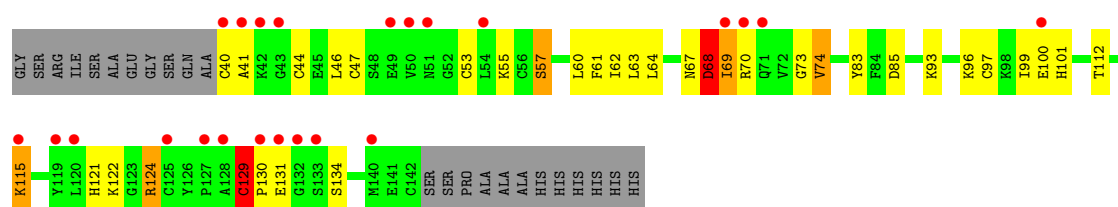
• Molecule 2: R-SPONDIN-1



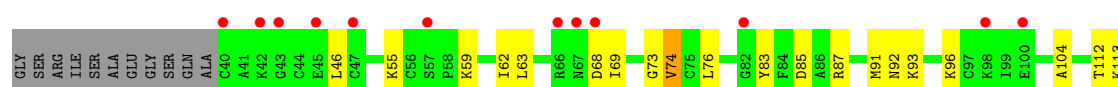
• Molecule 2: R-SPONDIN-1

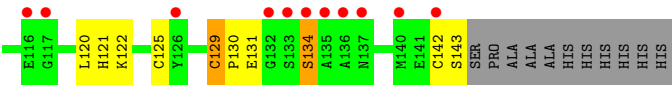


• Molecule 2: R-SPONDIN-1



• Molecule 2: R-SPONDIN-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.36Å 111.30Å 130.61Å 90.00° 109.19° 90.00°	Depositor
Resolution (Å)	28.90 – 3.20 28.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (28.90-3.20) 97.1 (28.90-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.18Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.246 , 0.290 0.249 , 0.294	Depositor DCC
R_{free} test set	2660 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 80.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17925	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.84% 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: NAG

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	0.27	0/3734	0.58	3/5085 (0.1%)
1	B	0.27	0/3752	0.55	2/5109 (0.0%)
1	E	0.27	0/3753	0.61	1/5109 (0.0%)
1	F	0.27	0/3718	0.57	1/5062 (0.0%)
2	C	0.29	0/794	0.59	0/1066
2	D	0.27	0/800	0.54	0/1074
2	G	0.27	0/794	0.55	0/1066
2	H	0.29	0/800	0.56	0/1074
All	All	0.27	0/18145	0.57	7/24645 (0.0%)

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
3	A	1	0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	533	LEU	CA-CB-CG	6.58	130.44	115.30
1	A	82	LEU	CA-CB-CG	6.57	130.40	115.30
1	B	442	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	433	LEU	CA-CB-CG	5.76	128.56	115.30
1	E	354	LEU	CA-CB-CG	5.58	128.14	115.30
1	F	357	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	442	LEU	CA-CB-CG	5.14	127.12	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1208	NAG	C1

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	3653	0	3652	74	9
1	B	3671	0	3685	94	0
1	E	3672	0	3674	142	1
1	F	3637	0	3652	96	8
2	C	778	0	744	22	0
2	D	784	0	749	16	0
2	G	778	0	744	21	0
2	H	784	0	749	20	0
3	A	56	0	50	0	0
3	B	28	0	25	0	0
3	E	28	0	25	0	0
4	B	28	0	26	2	0
4	E	14	0	13	1	0
4	F	14	0	13	0	0
All	All	17925	0	17801	467	9

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 13.

All (467) 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:F:408:ASN:HD21	1:F:410:ILE:HG13	1.23	1.01
1:E:343:LEU:HD11	1:E:368:PRO:HG3	1.53	0.87
1:A:282:SER:HA	1:A:306:GLU:HG3	1.58	0.86
1:E:259:LEU:HD13	1:E:262:LEU:HD11	1.57	0.85
1:B:107:LYS:HD2	1:B:132:GLU:HB2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:SER:HB3	1:E:449:LYS:HD2	1.60	0.81
1:E:153:VAL:HG21	1:E:178:PRO:HG3	1.61	0.80
1:E:60:LEU:HD12	1:E:61:PRO:HD2	1.64	0.80
1:A:146:ASP:OD2	2:C:87:ARG:NH1	2.16	0.79
1:B:428:ASP:OD1	1:B:430:SER:OG	2.00	0.78
1:E:304:LEU:HD13	1:E:307:LEU:HD21	1.64	0.78
1:B:100:ASN:O	1:B:124:ASN:ND2	2.17	0.78
1:F:298:ARG:HB2	1:F:322:PRO:HA	1.65	0.78
1:A:177:ILE:HD13	1:A:205:ALA:HB1	1.66	0.77
1:E:316:SER:O	1:E:339:GLN:NE2	2.18	0.76
1:B:182:PHE:HB3	1:B:209:LEU:HD11	1.68	0.76
1:E:324:LEU:HD13	1:E:330:LEU:HD21	1.67	0.75
1:E:213:VAL:HG13	1:E:214:VAL:HG13	1.68	0.74
1:E:161:LEU:HD11	1:E:185:LEU:HD23	1.71	0.73
1:E:301:PHE:CE1	1:E:322:PRO:HB3	2.22	0.73
1:E:206:PHE:HB3	1:E:209:LEU:HD11	1.69	0.73
1:A:182:PHE:HB3	1:A:209:LEU:HD11	1.70	0.72
1:F:104:TYR:HH	1:F:131:THR:HG1	1.37	0.72
1:E:182:PHE:HA	1:E:185:LEU:HD12	1.71	0.72
1:F:357:LEU:HD11	1:F:379:ILE:HG12	1.72	0.71
1:E:302:GLN:HE22	1:E:325:THR:HB	1.54	0.71
2:H:130:PRO:HA	2:H:131:GLU:HB2	1.72	0.71
1:F:60:LEU:HG	1:F:82:LEU:HD11	1.72	0.71
1:B:480:CYS:SG	2:C:66:ARG:NH2	2.63	0.71
1:B:480:CYS:HB3	2:C:66:ARG:HH12	1.56	0.70
1:E:57:LEU:HB2	1:E:76:ASN:OD1	1.92	0.69
1:E:140:LEU:HD11	1:E:161:LEU:HB2	1.74	0.68
2:G:130:PRO:HA	2:G:131:GLU:HB2	1.76	0.68
1:F:82:LEU:HD13	1:F:85:PRO:HA	1.75	0.68
1:A:92:LEU:HD21	1:A:95:LEU:HB3	1.76	0.68
1:A:428:ASP:OD1	1:A:430:SER:OG	2.11	0.67
2:C:70:ARG:NH2	2:C:71:GLN:O	2.27	0.67
1:E:439:ILE:HD11	1:E:464:ASN:HB3	1.77	0.67
1:F:295:PHE:HB2	1:F:317:GLN:HB2	1.76	0.67
1:B:153:VAL:O	1:F:298:ARG:NH2	2.28	0.66
1:B:66:VAL:HG22	1:B:67:PHE:H	1.61	0.66
1:E:413:ILE:HG21	1:E:438:PRO:HG3	1.76	0.66
2:G:83:TYR:CD1	2:G:96:LYS:HA	2.30	0.66
1:F:343:LEU:H	1:F:343:LEU:HD12	1.60	0.66
1:B:107:LYS:NZ	1:B:131:THR:OG1	2.28	0.66
1:E:233:LEU:HD23	1:E:256:LEU:HD21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:ASP:N	1:F:170:ASP:OD1	2.26	0.66
1:E:137:LEU:O	1:E:139:SER:N	2.29	0.66
1:A:258:ASN:OD1	1:A:258:ASN:N	2.30	0.65
1:B:102:LEU:HG	1:B:124:ASN:HD22	1.62	0.65
1:E:237:GLU:HA	1:E:259:LEU:HA	1.78	0.64
1:B:334:THR:HB	1:B:358:ASP:HB3	1.79	0.64
1:E:376:LEU:HD23	1:E:379:ILE:HD11	1.80	0.64
2:C:114:CYS:H	2:C:120:LEU:HD12	1.62	0.64
2:D:130:PRO:HA	2:D:131:GLU:CG	2.28	0.64
1:F:379:ILE:HD12	1:F:400:LEU:HD21	1.80	0.64
2:H:91:MET:SD	2:H:93:LYS:NZ	2.71	0.64
1:E:177:ILE:HD11	1:E:201:ILE:HG12	1.80	0.64
1:B:155:PRO:HA	1:B:180:GLN:HE21	1.64	0.63
2:C:51:ASN:HA	2:C:70:ARG:NH2	2.14	0.62
1:A:132:GLU:O	1:A:134:LEU:N	2.33	0.62
1:F:107:LYS:H	1:F:107:LYS:HD2	1.62	0.62
1:E:233:LEU:HD13	1:E:233:LEU:H	1.65	0.62
1:F:386:ILE:O	1:F:408:ASN:ND2	2.33	0.62
1:F:144:ARG:NH1	2:H:85:ASP:OD2	2.33	0.62
1:F:306:GLU:O	1:F:308:ARG:NH1	2.34	0.61
1:E:158:PHE:O	1:E:161:LEU:HG	2.01	0.61
1:F:327:THR:OG1	1:F:327:THR:O	2.14	0.61
1:B:201:ILE:HG22	1:B:229:CYS:HB2	1.82	0.61
1:A:425:ILE:HB	1:A:446:THR:HG22	1.81	0.60
1:B:104:TYR:OH	1:B:107:LYS:NZ	2.31	0.60
1:E:380:ASP:HA	1:E:404:ASN:HB3	1.83	0.60
1:F:223:HIS:NE2	1:F:247:ASP:OD2	2.34	0.60
1:E:318:ILE:HG22	1:E:340:ILE:HD11	1.83	0.60
1:F:101:ALA:HB1	1:F:125:GLN:HE22	1.66	0.60
1:B:180:GLN:HE22	1:F:298:ARG:HH21	1.49	0.60
1:F:137:LEU:O	1:F:139:SER:N	2.35	0.60
1:E:327:THR:O	1:E:327:THR:OG1	2.15	0.60
1:A:137:LEU:O	1:A:139:SER:N	2.35	0.60
1:F:148:ASN:HB2	1:F:150:ILE:HG22	1.83	0.60
1:F:171:ASP:OD2	2:H:59:LYS:NZ	2.34	0.60
1:B:425:ILE:HG13	1:B:426:LYS:HG3	1.84	0.60
1:E:446:THR:HG23	1:E:447:HIS:ND1	2.17	0.60
1:F:66:VAL:HG22	1:F:67:PHE:H	1.66	0.60
2:D:130:PRO:HA	2:D:131:GLU:HG2	1.84	0.59
1:E:236:LEU:HD22	1:E:256:LEU:HD13	1.82	0.59
1:E:356:VAL:HG13	1:E:378:LYS:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:LEU:HD21	1:E:250:PRO:HB3	1.84	0.59
1:E:449:LYS:HG2	1:E:472:GLU:HG3	1.85	0.59
1:B:147:ALA:HB2	2:D:87:ARG:HH12	1.67	0.58
1:A:66:VAL:HG22	1:A:67:PHE:H	1.69	0.58
1:F:43:ASP:OD1	1:F:49:ARG:HG3	2.02	0.58
1:E:137:LEU:O	1:E:140:LEU:HD12	2.03	0.58
1:E:351:LEU:HD23	1:E:354:LEU:HD11	1.85	0.58
1:B:473:MET:HG3	1:B:474:PRO:HD2	1.85	0.58
1:E:66:VAL:HG22	1:E:67:PHE:H	1.69	0.58
2:G:122:LYS:NZ	2:G:124:ARG:HH12	2.03	0.57
1:A:144:ARG:NH1	2:C:85:ASP:OD2	2.37	0.57
1:E:209:LEU:HD13	1:E:212:LEU:HD22	1.87	0.57
1:A:473:MET:HG3	1:A:474:PRO:HD2	1.86	0.57
1:B:449:LYS:HG2	1:B:472:GLU:HG3	1.86	0.57
1:F:446:THR:HA	1:F:468:LEU:HA	1.87	0.57
1:B:465:PHE:HB3	1:B:468:LEU:HD12	1.86	0.57
1:F:107:LYS:N	1:F:107:LYS:HD2	2.20	0.57
1:A:465:PHE:HB3	1:A:468:LEU:HD12	1.87	0.57
1:F:43:ASP:OD2	1:F:69:SER:OG	2.23	0.57
1:B:327:THR:O	1:B:327:THR:OG1	2.19	0.56
1:F:465:PHE:HB3	1:F:468:LEU:HD12	1.87	0.56
1:A:201:ILE:HG22	1:A:229:CYS:HB2	1.88	0.56
1:F:131:THR:O	1:F:135:GLN:NE2	2.39	0.56
1:F:397:LEU:HD13	1:F:400:LEU:HD22	1.87	0.56
1:E:302:GLN:NE2	1:E:325:THR:O	2.39	0.56
1:F:351:LEU:HB3	1:F:354:LEU:HD12	1.88	0.56
2:D:121:HIS:NE2	2:D:130:PRO:HG2	2.21	0.56
1:F:49:ARG:HG2	1:F:70:TYR:HB3	1.87	0.56
1:E:43:ASP:O	1:E:45:ARG:N	2.38	0.56
1:A:234:HIS:O	1:A:258:ASN:ND2	2.38	0.56
1:E:140:LEU:HD11	1:E:161:LEU:CB	2.36	0.56
1:F:74:SER:O	1:F:76:ASN:ND2	2.39	0.56
2:G:130:PRO:HA	2:G:131:GLU:CB	2.36	0.56
1:E:458:SER:O	1:E:478:GLN:NE2	2.37	0.56
1:E:348:CYS:HB2	1:E:372:VAL:HG23	1.88	0.56
1:B:183:ARG:O	1:B:208:ASN:ND2	2.39	0.55
2:G:64:LEU:HG	2:G:93:LYS:HE3	1.87	0.55
2:D:59:LYS:HE2	2:D:87:ARG:HH22	1.71	0.55
1:F:178:PRO:HD2	1:F:182:PHE:HE2	1.71	0.55
1:A:334:THR:HB	1:A:358:ASP:HB3	1.87	0.55
1:A:420:THR:O	1:A:420:THR:OG1	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LEU:HD13	1:A:364:LEU:HD21	1.88	0.55
1:E:237:GLU:OE2	2:G:124:ARG:NH2	2.40	0.55
1:B:442:LEU:HD13	1:B:445:LEU:HD21	1.89	0.55
1:E:282:SER:HA	1:E:306:GLU:HG3	1.89	0.55
2:G:40:CYS:SG	2:G:41:ALA:N	2.80	0.55
1:F:104:TYR:HE1	1:F:130:PRO:HA	1.72	0.55
1:E:161:LEU:O	1:E:163:SER:N	2.39	0.54
1:F:386:ILE:HG23	1:F:408:ASN:ND2	2.22	0.54
1:A:391:VAL:HG22	1:A:414:HIS:CG	2.42	0.54
1:B:425:ILE:HB	1:B:446:THR:HG22	1.90	0.54
2:C:51:ASN:HA	2:C:70:ARG:HH22	1.71	0.54
2:G:47:CYS:HA	2:G:53:CYS:HA	1.89	0.54
2:H:63:LEU:HD11	2:H:83:TYR:CE2	2.43	0.54
1:B:82:LEU:HD13	1:B:85:PRO:HA	1.89	0.54
1:A:144:ARG:HG2	1:A:168:TRP:CE3	2.43	0.53
1:A:351:LEU:HG	1:A:354:LEU:HD22	1.91	0.53
1:B:391:VAL:HG22	1:B:414:HIS:CD2	2.43	0.53
1:E:280:ASN:O	1:E:283:LEU:HD12	2.08	0.53
1:A:231:ASP:HA	1:A:255:THR:HG21	1.90	0.53
1:B:137:LEU:O	1:B:139:SER:N	2.42	0.53
1:B:197:LYS:HD3	1:B:221:ARG:HH12	1.74	0.53
1:E:253:ILE:HD12	1:E:256:LEU:HD12	1.88	0.53
1:F:213:VAL:HG21	2:H:122:LYS:HB2	1.89	0.53
1:B:180:GLN:NE2	1:F:298:ARG:HH21	2.06	0.53
1:B:180:GLN:N	1:B:180:GLN:OE1	2.41	0.53
1:B:233:LEU:HD13	1:B:233:LEU:H	1.74	0.53
1:E:82:LEU:HD13	1:E:85:PRO:HA	1.91	0.53
1:E:457:GLN:HG2	1:E:475:TYR:HE2	1.74	0.53
1:B:237:GLU:OE2	2:D:124:ARG:NH2	2.42	0.52
2:H:130:PRO:HA	2:H:131:GLU:CB	2.37	0.52
1:A:389:ILE:HG23	1:A:393:THR:HG21	1.90	0.52
1:E:144:ARG:HG2	1:E:168:TRP:CE3	2.45	0.52
2:C:126:TYR:N	2:C:126:TYR:CD1	2.77	0.52
1:E:144:ARG:NH2	1:E:146:ASP:OD2	2.43	0.52
1:A:327:THR:O	1:A:327:THR:OG1	2.26	0.52
2:C:130:PRO:HA	2:C:131:GLU:CB	2.40	0.52
1:A:100:ASN:O	1:A:124:ASN:ND2	2.43	0.52
1:B:476:ALA:HB2	1:B:543:PRO:HB3	1.92	0.52
1:B:57:LEU:HB3	1:B:76:ASN:HB3	1.92	0.51
1:E:404:ASN:HA	1:E:428:ASP:OD1	2.09	0.51
1:A:177:ILE:HD12	1:A:206:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:425:ILE:HG13	1:F:426:LYS:HG3	1.93	0.51
1:E:60:LEU:HD12	1:E:61:PRO:CD	2.38	0.51
1:F:144:ARG:HG2	1:F:168:TRP:CE3	2.44	0.51
2:H:134:SER:HA	2:H:143:SER:HB3	1.92	0.51
1:B:376:LEU:HD23	1:B:379:ILE:HD11	1.91	0.51
1:E:329:ASN:ND2	1:E:329:ASN:O	2.38	0.51
2:H:121:HIS:CE1	2:H:130:PRO:HG2	2.45	0.51
1:F:214:VAL:HG22	1:F:238:THR:HG22	1.92	0.51
1:F:340:ILE:HG22	1:F:362:ASN:OD1	2.11	0.51
1:A:353:ASN:HA	1:A:375:LYS:HD2	1.92	0.51
1:E:425:ILE:HB	1:E:446:THR:HG22	1.93	0.51
1:E:302:GLN:HG3	1:E:303:HIS:ND1	2.25	0.50
1:B:480:CYS:CB	2:C:66:ARG:HH12	2.24	0.50
1:A:33:GLY:O	1:A:65:SER:HB3	2.11	0.50
1:A:41:GLU:OE1	1:A:42:PRO:HD2	2.11	0.50
1:E:104:TYR:OH	1:E:131:THR:OG1	2.25	0.50
1:E:64:LEU:HD23	1:E:89:LEU:HD21	1.93	0.50
1:F:348:CYS:HB2	1:F:372:VAL:HB	1.94	0.50
1:A:96:ARG:HA	1:A:120:MET:HB2	1.93	0.50
1:B:311:THR:HG22	1:B:334:THR:HG23	1.94	0.50
1:B:442:LEU:O	1:B:442:LEU:HD12	2.12	0.50
1:F:340:ILE:HD11	1:F:342:SER:O	2.12	0.50
1:F:386:ILE:HG13	1:F:387:TYR:N	2.26	0.50
1:E:260:LYS:NZ	1:E:282:SER:O	2.31	0.50
1:F:96:ARG:HA	1:F:120:MET:HB2	1.92	0.50
1:F:318:ILE:HG13	1:F:338:ALA:HB1	1.93	0.50
1:B:437:PHE:HE2	1:B:456:LEU:HD11	1.75	0.50
1:B:147:ALA:HB2	2:D:87:ARG:NH1	2.27	0.50
2:G:121:HIS:NE2	2:G:122:LYS:HE3	2.26	0.50
2:D:45:GLU:OE2	2:D:58:PRO:HD3	2.12	0.50
2:C:64:LEU:HD22	2:C:93:LYS:HE3	1.94	0.49
1:E:158:PHE:HB3	1:E:161:LEU:HD21	1.93	0.49
1:E:389:ILE:HB	1:E:413:ILE:HD13	1.94	0.49
1:B:343:LEU:HD13	1:B:364:LEU:HD21	1.94	0.49
1:E:231:ASP:HA	1:E:255:THR:HG21	1.95	0.49
1:A:82:LEU:HD12	1:A:83:PRO:HD2	1.93	0.49
1:F:95:LEU:HD21	1:F:97:LEU:HD22	1.93	0.49
1:A:296:VAL:HG11	1:A:301:PHE:HE1	1.77	0.49
1:B:169:LEU:HB2	1:B:193:LEU:HD23	1.94	0.49
2:G:121:HIS:NE2	2:G:130:PRO:HG2	2.28	0.49
1:B:194:ALA:O	1:B:196:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:GLU:O	1:E:134:LEU:N	2.45	0.49
1:A:192:THR:HG23	1:A:216:HIS:HB2	1.95	0.49
2:C:116:GLU:HA	2:C:140:MET:SD	2.52	0.49
1:E:387:TYR:HA	1:E:410:ILE:HA	1.93	0.49
2:C:40:CYS:SG	2:C:41:ALA:N	2.86	0.49
1:E:213:VAL:HG23	1:E:237:GLU:HG3	1.94	0.49
1:F:132:GLU:O	1:F:134:LEU:N	2.46	0.49
1:A:92:LEU:HD23	1:A:94:GLU:H	1.77	0.49
1:E:351:LEU:HB3	1:E:354:LEU:HD11	1.95	0.49
1:E:457:GLN:O	1:E:477:TYR:OH	2.25	0.49
1:F:233:LEU:HD13	1:F:233:LEU:H	1.78	0.49
1:F:320:GLU:HA	1:F:340:ILE:HD13	1.95	0.49
2:G:67:ASN:HB3	2:G:70:ARG:HE	1.78	0.49
1:B:170:ASP:OD1	1:B:170:ASP:N	2.45	0.49
1:F:389:ILE:HG23	1:F:393:THR:HG21	1.94	0.49
1:F:334:THR:HB	1:F:358:ASP:HB3	1.94	0.48
1:B:102:LEU:HD13	1:B:105:ILE:HD11	1.95	0.48
2:H:63:LEU:O	2:H:73:GLY:HA2	2.14	0.48
1:E:380:ASP:OD1	1:E:404:ASN:ND2	2.47	0.48
1:E:81:LEU:HD21	1:E:102:LEU:HD13	1.94	0.48
1:B:414:HIS:CG	1:B:415:PRO:HD2	2.49	0.48
2:C:126:TYR:N	2:C:126:TYR:HD1	2.11	0.48
1:E:283:LEU:HD11	1:E:304:LEU:HB3	1.95	0.48
1:E:180:GLN:OE1	1:E:180:GLN:N	2.42	0.48
2:G:97:CYS:SG	2:G:99:ILE:HD12	2.54	0.48
2:C:121:HIS:CE1	2:C:130:PRO:HG2	2.49	0.48
1:A:165:ARG:HA	1:A:188:LEU:HA	1.96	0.47
1:F:386:ILE:HD11	1:F:388:GLU:O	2.14	0.47
1:A:74:SER:O	1:A:76:ASN:ND2	2.46	0.47
1:B:104:TYR:HE1	1:B:130:PRO:HA	1.79	0.47
1:E:140:LEU:HD13	1:E:140:LEU:O	2.13	0.47
2:G:62:ILE:HA	2:G:74:VAL:O	2.14	0.47
1:E:465:PHE:HB3	1:E:468:LEU:HD13	1.95	0.47
1:A:425:ILE:HG13	1:A:426:LYS:HG3	1.96	0.47
1:A:45:ARG:HD3	1:A:46:MET:H	1.79	0.47
1:B:104:TYR:OH	1:B:131:THR:OG1	2.20	0.47
1:B:208:ASN:OD1	4:B:1208:NAG:N2	2.48	0.47
1:F:147:ALA:HA	1:F:171:ASP:HB3	1.96	0.47
2:H:83:TYR:CD1	2:H:96:LYS:HA	2.49	0.47
1:B:165:ARG:HA	1:B:188:LEU:HA	1.97	0.47
1:E:33:GLY:O	1:E:65:SER:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:ILE:HG13	1:E:426:LYS:HG3	1.97	0.47
1:F:150:ILE:HD12	1:F:152:TYR:H	1.80	0.47
1:B:344:PRO:O	1:B:347:VAL:HG22	2.15	0.47
1:B:75:MET:N	1:B:75:MET:SD	2.87	0.47
1:E:388:GLU:N	1:E:388:GLU:OE1	2.48	0.47
1:A:129:VAL:HG21	1:A:153:VAL:HG13	1.96	0.47
4:B:1077:NAG:O7	4:B:1077:NAG:O3	2.30	0.47
1:F:197:LYS:HD3	1:F:221:ARG:HH12	1.79	0.47
1:F:333:LEU:O	1:F:357:LEU:HA	2.15	0.47
1:E:75:MET:SD	1:E:75:MET:N	2.87	0.47
1:B:392:ASP:HA	1:B:395:GLN:HG2	1.97	0.46
1:E:189:GLN:O	1:E:213:VAL:HG12	2.15	0.46
1:E:203:ASP:HA	1:E:229:CYS:HA	1.96	0.46
1:E:60:LEU:HD13	1:E:73:LEU:HD11	1.96	0.46
1:A:306:GLU:O	1:A:308:ARG:NH1	2.48	0.46
2:D:119:TYR:HB3	2:D:142:CYS:SG	2.55	0.46
1:E:368:PRO:HD2	1:E:370:PHE:CE2	2.50	0.46
1:E:391:VAL:HG22	1:E:414:HIS:CD2	2.50	0.46
1:E:463:GLU:O	1:E:464:ASN:HB2	2.14	0.46
1:E:97:LEU:HD12	1:E:100:ASN:ND2	2.30	0.46
1:F:72:ASP:HA	1:F:96:ARG:HB2	1.97	0.46
2:G:124:ARG:HG2	2:G:124:ARG:H	1.52	0.46
1:B:105:ILE:HA	1:B:106:PRO:HD2	1.76	0.46
1:B:262:LEU:HD22	1:B:264:PHE:HD1	1.81	0.46
1:E:153:VAL:HG21	1:E:178:PRO:CG	2.39	0.46
1:E:373:CYS:O	1:E:376:LEU:HD13	2.16	0.46
1:F:40:CYS:HB3	1:F:48:LEU:HD21	1.97	0.46
1:E:194:ALA:O	1:E:196:ASN:ND2	2.48	0.46
1:B:411:ALA:HA	1:B:433:LEU:O	2.16	0.46
1:E:201:ILE:HG22	1:E:229:CYS:HB2	1.97	0.46
1:E:374:GLN:HG3	1:E:375:LYS:HG2	1.98	0.46
1:B:164:LEU:HD23	1:B:185:LEU:HD22	1.98	0.46
1:E:434:LEU:O	1:E:455:ALA:HB3	2.16	0.46
1:A:75:MET:N	1:A:75:MET:SD	2.89	0.46
1:B:367:LEU:HD11	1:B:386:ILE:HD13	1.97	0.45
1:E:80:GLN:HG2	1:E:83:PRO:HD3	1.98	0.45
2:G:122:LYS:HZ2	2:G:124:ARG:HH12	1.64	0.45
2:H:63:LEU:HD11	2:H:83:TYR:HE2	1.80	0.45
1:E:220:ASN:N	1:E:244:ASN:OD1	2.45	0.45
1:E:40:CYS:HB3	1:E:48:LEU:HD21	1.97	0.45
1:E:457:GLN:HB3	2:H:91:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:457:GLN:HG2	1:E:475:TYR:CE2	2.52	0.45
1:A:82:LEU:CD1	1:A:84:ASN:H	2.29	0.45
1:B:393:THR:HG22	1:B:394:PHE:CD2	2.51	0.45
1:B:53:SER:HA	1:B:76:ASN:HD21	1.81	0.45
1:F:134:LEU:O	1:F:161:LEU:HD11	2.17	0.45
1:F:171:ASP:HB2	2:H:87:ARG:HD3	1.97	0.45
1:B:359:LEU:HB2	1:B:381:LEU:HD23	1.98	0.45
1:F:393:THR:HG23	1:F:394:PHE:CD2	2.52	0.45
1:F:165:ARG:O	1:F:166:HIS:ND1	2.49	0.45
1:F:459:LEU:HA	1:F:459:LEU:HD23	1.72	0.45
1:A:324:LEU:HD22	1:A:330:LEU:HD11	1.98	0.45
1:B:120:MET:HA	1:B:144:ARG:HB2	1.98	0.45
1:B:78:ILE:O	1:B:78:ILE:HG13	2.16	0.45
1:E:259:LEU:HD22	1:E:262:LEU:HD21	1.98	0.45
1:B:203:ASP:HA	1:B:229:CYS:HA	1.98	0.45
1:E:165:ARG:HA	1:E:188:LEU:HA	1.99	0.45
1:E:369:SER:C	1:E:371:SER:H	2.21	0.45
1:F:75:MET:N	1:F:75:MET:SD	2.90	0.45
2:H:87:ARG:HG3	2:H:92:ASN:OD1	2.17	0.45
1:B:437:PHE:CD2	1:B:456:LEU:HD21	2.52	0.45
1:F:43:ASP:N	1:F:43:ASP:OD1	2.49	0.45
1:A:367:LEU:HD11	1:A:386:ILE:HD13	1.99	0.44
1:E:220:ASN:HB2	1:E:244:ASN:HD21	1.83	0.44
2:H:104:ALA:HB3	2:H:113:LYS:HG2	1.99	0.44
1:A:192:THR:HG22	1:A:194:ALA:H	1.83	0.44
1:A:223:HIS:NE2	1:A:247:ASP:OD2	2.51	0.44
2:C:130:PRO:HA	2:C:131:GLU:CG	2.47	0.44
1:F:223:HIS:CD2	1:F:223:HIS:O	2.71	0.44
1:F:324:LEU:HD22	1:F:330:LEU:HD11	1.99	0.44
1:E:110:PHE:HA	1:E:113:LEU:HD23	1.99	0.44
1:A:144:ARG:NH2	1:A:146:ASP:OD2	2.51	0.44
1:A:295:PHE:HB2	1:A:317:GLN:HB2	1.99	0.44
1:A:194:ALA:O	1:A:196:ASN:ND2	2.50	0.44
1:E:265:HIS:HB2	1:E:289:TYR:O	2.18	0.44
1:F:107:LYS:HG3	1:F:132:GLU:HB2	1.99	0.44
1:A:220:ASN:HB3	1:A:221:ARG:H	1.59	0.44
2:C:58:PRO:C	2:C:59:LYS:HD2	2.38	0.44
1:E:177:ILE:HD11	1:E:201:ILE:HA	1.98	0.44
1:E:59:GLU:HB3	1:E:82:LEU:HD21	1.99	0.44
1:A:153:VAL:HA	1:A:154:PRO:HD2	1.86	0.44
1:A:78:ILE:HB	1:A:100:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:HG	1:A:84:ASN:H	1.82	0.44
1:E:249:PHE:HA	1:E:250:PRO:HD3	1.81	0.44
1:E:122:GLN:HG2	1:E:144:ARG:CZ	2.47	0.44
1:E:356:VAL:HG22	1:E:378:LYS:HE3	2.00	0.44
1:F:87:PRO:C	1:F:89:LEU:H	2.21	0.44
1:A:57:LEU:HB2	1:A:76:ASN:HB3	1.99	0.43
1:B:87:PRO:HB3	1:B:112:GLY:HA3	2.00	0.43
1:B:376:LEU:HD12	1:B:376:LEU:HA	1.83	0.43
1:E:394:PHE:CD2	1:E:421:LEU:HD11	2.53	0.43
1:B:43:ASP:O	1:B:45:ARG:N	2.51	0.43
1:E:36:THR:O	1:E:37:HIS:HB2	2.18	0.43
1:F:246:LEU:HD23	1:F:250:PRO:HG3	2.00	0.43
1:B:131:THR:O	1:B:135:GLN:NE2	2.51	0.43
1:B:192:THR:HG22	2:D:106:PHE:HZ	1.83	0.43
1:E:233:LEU:CD2	1:E:256:LEU:HD21	2.46	0.43
1:F:389:ILE:HB	1:F:413:ILE:HD13	1.99	0.43
1:A:352:PRO:C	1:A:354:LEU:H	2.22	0.43
1:E:152:TYR:CD2	1:E:154:PRO:HD3	2.54	0.43
1:B:182:PHE:HA	1:B:185:LEU:HD12	2.00	0.43
1:B:216:HIS:HA	1:B:240:ASP:HB3	2.01	0.43
1:F:178:PRO:HD2	1:F:182:PHE:CE2	2.53	0.43
1:F:60:LEU:H	1:F:82:LEU:HD21	1.84	0.43
1:B:201:ILE:HG13	1:B:222:ILE:HD12	2.01	0.43
1:F:301:PHE:O	1:F:327:THR:HG21	2.18	0.43
2:G:115:LYS:HA	2:G:115:LYS:HD3	1.82	0.43
1:B:348:CYS:HB2	1:B:372:VAL:HB	2.00	0.43
1:F:361:TYR:O	1:F:361:TYR:HD1	2.02	0.43
2:G:121:HIS:HB2	2:G:129:CYS:HB2	2.00	0.43
1:A:301:PHE:O	1:A:327:THR:HG21	2.19	0.43
1:B:270:ARG:HE	1:B:270:ARG:HB3	1.56	0.43
2:C:68:ASP:O	2:C:69:ILE:HG22	2.19	0.43
2:G:68:ASP:O	2:G:69:ILE:HG22	2.18	0.43
1:E:540:GLN:NE2	1:E:541:CYS:O	2.52	0.43
1:A:390:LYS:O	1:A:393:THR:HG22	2.18	0.43
1:B:213:VAL:HG12	1:B:214:VAL:HG23	2.00	0.43
1:E:260:LYS:HZ1	1:E:284:ILE:HD11	1.84	0.43
1:E:73:LEU:HD22	1:E:76:ASN:ND2	2.33	0.43
1:F:391:VAL:HG22	1:F:414:HIS:CD2	2.54	0.43
1:F:41:GLU:CD	1:F:42:PRO:HD2	2.40	0.43
1:E:260:LYS:HA	1:E:283:LEU:HA	2.00	0.42
1:E:304:LEU:HD13	1:E:307:LEU:CD2	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ARG:HG3	1:B:309:THR:N	2.33	0.42
2:D:61:PHE:CZ	2:D:85:ASP:HB3	2.54	0.42
1:B:248:GLU:OE1	1:E:270:ARG:NE	2.52	0.42
1:E:333:LEU:HD23	1:E:351:LEU:HD21	2.00	0.42
1:E:59:GLU:HA	1:E:78:ILE:HG23	2.01	0.42
1:F:284:ILE:O	1:F:307:LEU:HD12	2.19	0.42
2:H:121:HIS:ND1	2:H:130:PRO:HG2	2.34	0.42
2:D:121:HIS:NE2	2:D:122:LYS:HE2	2.34	0.42
1:E:96:ARG:HA	1:E:120:MET:HB2	2.00	0.42
1:A:416:ASN:HA	1:A:440:THR:HG21	2.02	0.42
1:B:231:ASP:HA	1:B:255:THR:HG21	2.02	0.42
1:E:87:PRO:HB3	1:E:112:GLY:HA3	2.02	0.42
1:A:324:LEU:HD13	1:A:351:LEU:HD11	2.01	0.42
2:D:59:LYS:HE2	2:D:87:ARG:NH2	2.34	0.42
1:E:177:ILE:HD13	1:E:202:PRO:HD2	2.01	0.42
1:E:351:LEU:CD2	1:E:354:LEU:HD11	2.48	0.42
1:E:426:LYS:HA	1:E:447:HIS:HB2	2.02	0.42
2:D:130:PRO:HB3	2:D:132:GLY:N	2.35	0.42
1:E:97:LEU:HA	1:E:97:LEU:HD12	1.93	0.42
1:F:183:ARG:HA	1:F:208:ASN:HB2	2.02	0.42
1:A:105:ILE:HA	1:A:106:PRO:HD2	1.71	0.42
1:F:33:GLY:O	1:F:65:SER:HB3	2.18	0.42
2:G:61:PHE:CZ	2:G:85:ASP:HB3	2.54	0.42
1:A:321:PHE:HA	1:A:322:PRO:HD3	1.94	0.42
1:A:414:HIS:CG	1:A:415:PRO:HD2	2.55	0.42
1:A:154:PRO:HA	1:A:155:PRO:HD3	1.92	0.42
1:A:180:GLN:N	1:A:180:GLN:OE1	2.43	0.42
1:A:262:LEU:HD22	1:A:264:PHE:HD1	1.85	0.42
1:E:81:LEU:HD11	1:E:105:ILE:HD13	2.02	0.42
1:E:293:ILE:HD11	1:E:296:VAL:HG22	2.02	0.42
1:A:97:LEU:HB3	1:A:121:LEU:HD23	2.02	0.42
1:B:153:VAL:HA	1:B:154:PRO:HD2	1.83	0.42
2:C:63:LEU:O	2:C:73:GLY:HA2	2.20	0.42
1:E:343:LEU:CD1	1:E:368:PRO:HG3	2.38	0.42
1:B:463:GLU:O	1:B:464:ASN:HB2	2.20	0.41
1:B:75:MET:SD	1:B:99:GLY:HA3	2.60	0.41
1:E:53:SER:O	1:E:55:LEU:HD22	2.20	0.41
1:A:267:ASN:HB3	1:A:268:ASN:H	1.64	0.41
1:B:301:PHE:O	1:B:327:THR:HG21	2.20	0.41
1:E:100:ASN:O	1:E:102:LEU:HG	2.20	0.41
1:E:413:ILE:CG2	1:E:438:PRO:HG3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:PHE:HA	1:F:250:PRO:HD3	1.89	0.41
1:F:259:LEU:HD21	1:F:262:LEU:HG	2.02	0.41
1:A:59:GLU:HG2	1:A:82:LEU:HD13	2.02	0.41
1:B:127:ARG:C	1:B:150:ILE:HA	2.41	0.41
1:E:123:ASN:H	1:E:147:ALA:HB3	1.86	0.41
1:E:447:HIS:HA	1:E:470:VAL:HG13	2.03	0.41
1:E:43:ASP:C	1:E:45:ARG:N	2.74	0.41
2:H:83:TYR:HD1	2:H:96:LYS:HA	1.86	0.41
1:A:87:PRO:C	1:A:89:LEU:H	2.24	0.41
1:F:130:PRO:HB2	1:F:134:LEU:HD13	2.02	0.41
2:G:63:LEU:O	2:G:73:GLY:HA2	2.20	0.41
1:B:473:MET:HG2	1:B:478:GLN:CB	2.51	0.41
1:F:36:THR:O	1:F:37:HIS:HB2	2.21	0.41
1:F:71:LEU:HB2	1:F:92:LEU:HD21	2.03	0.41
2:H:62:ILE:HA	2:H:74:VAL:O	2.21	0.41
1:B:226:GLY:O	1:B:252:ALA:HB2	2.21	0.41
1:E:369:SER:O	1:E:371:SER:N	2.54	0.41
1:E:428:ASP:OD1	1:E:428:ASP:N	2.54	0.41
2:D:114:CYS:HB2	2:D:120:LEU:HD13	2.03	0.41
1:E:34:CYS:HA	1:E:35:PRO:HD3	1.94	0.41
1:E:79:SER:HB3	4:E:1077:NAG:O7	2.19	0.41
1:B:391:VAL:HG22	1:B:414:HIS:CG	2.56	0.41
1:B:94:GLU:OE2	1:B:96:ARG:NH2	2.54	0.41
2:C:130:PRO:HA	2:C:131:GLU:HB3	2.03	0.41
1:E:189:GLN:C	1:E:212:LEU:HD12	2.41	0.41
1:E:304:LEU:HD12	1:E:327:THR:HB	2.03	0.41
1:F:220:ASN:HB3	1:F:221:ARG:H	1.64	0.41
1:F:318:ILE:HG13	1:F:318:ILE:O	2.20	0.41
1:F:62:SER:C	1:F:64:LEU:H	2.23	0.41
1:B:445:LEU:HB2	1:B:446:THR:H	1.63	0.41
2:C:79:CYS:HB3	2:C:83:TYR:HB2	2.02	0.41
1:E:259:LEU:HD12	1:E:259:LEU:O	2.20	0.41
1:B:43:ASP:CG	1:B:44:GLY:H	2.22	0.40
1:B:97:LEU:HD12	1:B:100:ASN:ND2	2.36	0.40
1:F:158:PHE:CD2	1:F:185:LEU:HD11	2.56	0.40
1:A:148:ASN:HB2	1:A:150:ILE:HG22	2.04	0.40
1:A:233:LEU:H	1:A:233:LEU:HD13	1.84	0.40
1:B:102:LEU:HG	1:B:124:ASN:ND2	2.34	0.40
2:G:57:SER:HB3	2:G:60:LEU:HD12	2.04	0.40
1:A:45:ARG:HA	1:A:45:ARG:HD3	1.86	0.40
1:B:132:GLU:O	1:B:134:LEU:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:ASP:C	2:D:70:ARG:H	2.24	0.40
1:E:220:ASN:HB3	1:E:221:ARG:H	1.66	0.40
1:E:322:PRO:O	1:E:324:LEU:HD23	2.21	0.40
1:F:43:ASP:O	1:F:45:ARG:N	2.50	0.40
1:F:453:ASN:HB3	1:F:456:LEU:HB2	2.04	0.40
1:F:337:GLY:HA2	1:F:361:TYR:CD1	2.56	0.40
2:H:113:LYS:HG3	2:H:113:LYS:O	2.20	0.40
1:A:443:HIS:NE2	1:A:464:ASN:HA	2.36	0.40
1:B:348:CYS:HA	1:B:351:LEU:HB2	2.03	0.40
1:F:246:LEU:CD2	1:F:250:PRO:HG3	2.51	0.40
1:F:401:ARG:O	1:F:424:LEU:HD23	2.22	0.40

All (9) 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:A:531:GLU:OE2	1:F:67:PHE:CE2[1_454]	0.65	1.55
1:A:531:GLU:OE2	1:F:67:PHE:CZ[1_454]	0.80	1.40
1:A:531:GLU:CD	1:F:67:PHE:CE2[1_454]	1.47	0.73
1:A:531:GLU:CD	1:F:67:PHE:CZ[1_454]	1.67	0.53
1:A:531:GLU:OE2	1:F:67:PHE:CD2[1_454]	1.91	0.29
1:A:531:GLU:OE1	1:E:45:ARG:NH1[1_455]	1.95	0.25
1:A:531:GLU:OE2	1:F:67:PHE:CE1[1_454]	2.02	0.18
1:A:531:GLU:OE1	1:F:67:PHE:CZ[1_454]	2.19	0.01
1:A:531:GLU:CG	1:F:67:PHE:CE2[1_454]	2.19	0.01

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	462/539 (86%)	383 (83%)	69 (15%)	10 (2%)	8 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	465/539 (86%)	385 (83%)	67 (14%)	13 (3%)	6	34
1	E	464/539 (86%)	386 (83%)	61 (13%)	17 (4%)	4	26
1	F	460/539 (85%)	377 (82%)	69 (15%)	14 (3%)	5	32
2	C	101/126 (80%)	81 (80%)	16 (16%)	4 (4%)	3	24
2	D	102/126 (81%)	81 (79%)	16 (16%)	5 (5%)	2	19
2	G	101/126 (80%)	79 (78%)	18 (18%)	4 (4%)	3	24
2	H	102/126 (81%)	82 (80%)	15 (15%)	5 (5%)	2	19
All	All	2257/2660 (85%)	1854 (82%)	331 (15%)	72 (3%)	5	30

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	133	ALA
1	A	138	ARG
1	B	45	ARG
1	B	54	ASP
1	B	133	ALA
1	B	138	ARG
1	B	537	HIS
2	C	69	ILE
2	D	68	ASP
2	D	69	ILE
2	D	142	CYS
1	E	45	ARG
1	E	54	ASP
1	E	87	PRO
1	E	133	ALA
1	E	138	ARG
1	F	54	ASP
1	F	133	ALA
1	F	138	ARG
2	G	69	ILE
2	H	69	ILE
1	A	87	PRO
1	A	464	ASN
1	B	44	GLY
1	B	87	PRO
1	E	44	GLY
1	E	46	MET

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Mol	Chain	Res	Type
1	E	162	HIS
1	E	233	LEU
1	F	44	GLY
1	F	87	PRO
1	F	464	ASN
1	F	534	LYS
2	G	68	ASP
2	H	142	CYS
1	A	45	ARG
1	A	46	MET
1	A	444	GLY
1	B	46	MET
1	B	233	LEU
2	C	68	ASP
2	C	134	SER
2	D	134	SER
1	E	64	LEU
1	E	300	ALA
1	E	433	LEU
1	E	532	ASP
2	G	134	SER
2	H	68	ASP
1	A	233	LEU
1	B	464	ASN
1	F	45	ARG
1	F	233	LEU
1	F	444	GLY
1	B	444	GLY
2	C	129	CYS
2	D	129	CYS
1	E	370	PHE
1	E	464	ASN
1	F	162	HIS
2	G	129	CYS
2	H	129	CYS
2	H	134	SER
1	A	44	GLY
1	B	162	HIS
1	F	46	MET
1	E	444	GLY
1	F	66	VAL
1	F	368	PRO

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Mol	Chain	Res	Type
1	B	368	PRO
1	E	368	PRO

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	421/484 (87%)	378 (90%)	43 (10%)	8	34
1	B	423/484 (87%)	374 (88%)	49 (12%)	6	27
1	E	424/484 (88%)	362 (85%)	62 (15%)	3	17
1	F	420/484 (87%)	374 (89%)	46 (11%)	7	30
2	C	89/105 (85%)	77 (86%)	12 (14%)	4	20
2	D	90/105 (86%)	83 (92%)	7 (8%)	15	50
2	G	89/105 (85%)	77 (86%)	12 (14%)	4	20
2	H	90/105 (86%)	82 (91%)	8 (9%)	11	41
All	All	2046/2356 (87%)	1807 (88%)	239 (12%)	6	27

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	CYS
1	A	36	THR
1	A	46	MET
1	A	55	LEU
1	A	60	LEU
1	A	71	LEU
1	A	82	LEU
1	A	90	ARG
1	A	95	LEU
1	A	97	LEU
1	A	104	TYR
1	A	113	LEU
1	A	116	LEU

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Mol	Chain	Res	Type
1	A	118	VAL
1	A	122	GLN
1	A	135	GLN
1	A	145	LEU
1	A	150	ILE
1	A	165	ARG
1	A	179	VAL
1	A	233	LEU
1	A	239	LEU
1	A	253	ILE
1	A	258	ASN
1	A	270	ARG
1	A	287	HIS
1	A	298	ARG
1	A	312	LEU
1	A	327	THR
1	A	334	THR
1	A	351	LEU
1	A	357	LEU
1	A	372	VAL
1	A	374	GLN
1	A	420	THR
1	A	424	LEU
1	A	430	SER
1	A	440	THR
1	A	443	HIS
1	A	456	LEU
1	A	472	GLU
1	A	473	MET
1	A	533	LEU
1	B	32	ARG
1	B	34	CYS
1	B	55	LEU
1	B	57	LEU
1	B	64	LEU
1	B	71	LEU
1	B	78	ILE
1	B	92	LEU
1	B	97	LEU
1	B	104	TYR
1	B	116	LEU
1	B	118	VAL

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Mol	Chain	Res	Type
1	B	150	ILE
1	B	170	ASP
1	B	175	THR
1	B	186	SER
1	B	192	THR
1	B	227	LYS
1	B	233	LEU
1	B	238	THR
1	B	239	LEU
1	B	250	PRO
1	B	253	ILE
1	B	270	ARG
1	B	287	HIS
1	B	298	ARG
1	B	312	LEU
1	B	317	GLN
1	B	327	THR
1	B	334	THR
1	B	345	GLN
1	B	347	VAL
1	B	393	THR
1	B	412	ILE
1	B	420	THR
1	B	424	LEU
1	B	430	SER
1	B	437	PHE
1	B	442	LEU
1	B	443	HIS
1	B	445	LEU
1	B	456	LEU
1	B	472	GLU
1	B	473	MET
1	B	533	LEU
1	B	536	LEU
1	B	537	HIS
1	B	538	SER
1	B	539	VAL
2	C	46	LEU
2	C	57	SER
2	C	59	LYS
2	C	64	LEU
2	C	74	VAL

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Mol	Chain	Res	Type
2	C	112	THR
2	C	115	LYS
2	C	118	LEU
2	C	119	TYR
2	C	126	TYR
2	C	129	CYS
2	C	131	GLU
2	D	46	LEU
2	D	59	LYS
2	D	74	VAL
2	D	112	THR
2	D	124	ARG
2	D	129	CYS
2	D	131	GLU
1	E	34	CYS
1	E	45	ARG
1	E	55	LEU
1	E	60	LEU
1	E	78	ILE
1	E	81	LEU
1	E	86	LEU
1	E	90	ARG
1	E	92	LEU
1	E	97	LEU
1	E	107	LYS
1	E	113	LEU
1	E	116	LEU
1	E	118	VAL
1	E	122	GLN
1	E	140	LEU
1	E	150	ILE
1	E	153	VAL
1	E	161	LEU
1	E	186	SER
1	E	203	ASP
1	E	208	ASN
1	E	209	LEU
1	E	221	ARG
1	E	233	LEU
1	E	239	LEU
1	E	283	LEU
1	E	298	ARG

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Mol	Chain	Res	Type
1	E	301	PHE
1	E	304	LEU
1	E	307	LEU
1	E	310	LEU
1	E	312	LEU
1	E	313	ASN
1	E	316	SER
1	E	324	LEU
1	E	327	THR
1	E	329	ASN
1	E	330	LEU
1	E	339	GLN
1	E	357	LEU
1	E	359	LEU
1	E	364	LEU
1	E	366	ASP
1	E	372	VAL
1	E	377	GLN
1	E	381	LEU
1	E	410	ILE
1	E	420	THR
1	E	424	LEU
1	E	433	LEU
1	E	439	ILE
1	E	443	HIS
1	E	445	LEU
1	E	449	LYS
1	E	456	LEU
1	E	472	GLU
1	E	473	MET
1	E	484	VAL
1	E	533	LEU
1	E	537	HIS
1	E	540	GLN
1	F	34	CYS
1	F	39	HIS
1	F	43	ASP
1	F	47	LEU
1	F	50	VAL
1	F	55	LEU
1	F	57	LEU
1	F	64	LEU

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Mol	Chain	Res	Type
1	F	68	THR
1	F	97	LEU
1	F	107	LYS
1	F	116	LEU
1	F	118	VAL
1	F	127	ARG
1	F	134	LEU
1	F	137	LEU
1	F	150	ILE
1	F	162	HIS
1	F	170	ASP
1	F	192	THR
1	F	195	LEU
1	F	233	LEU
1	F	239	LEU
1	F	253	ILE
1	F	268	ASN
1	F	283	LEU
1	F	304	LEU
1	F	312	LEU
1	F	318	ILE
1	F	327	THR
1	F	329	ASN
1	F	334	THR
1	F	343	LEU
1	F	357	LEU
1	F	361	TYR
1	F	374	GLN
1	F	386	ILE
1	F	397	LEU
1	F	424	LEU
1	F	443	HIS
1	F	456	LEU
1	F	459	LEU
1	F	472	GLU
1	F	473	MET
1	F	536	LEU
1	F	538	SER
2	G	44	CYS
2	G	46	LEU
2	G	55	LYS
2	G	57	SER

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Mol	Chain	Res	Type
2	G	68	ASP
2	G	74	VAL
2	G	100	GLU
2	G	101	HIS
2	G	112	THR
2	G	115	LYS
2	G	124	ARG
2	G	129	CYS
2	H	46	LEU
2	H	55	LYS
2	H	74	VAL
2	H	76	LEU
2	H	112	THR
2	H	120	LEU
2	H	125	CYS
2	H	129	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	355	GLN
1	B	76	ASN
1	B	135	GLN
1	E	302	GLN
1	E	339	GLN
1	F	135	GLN

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](#)

8 carbohydrates 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	$\# Z > 2$
3	NAG	A	1077	1,3	14,14,15	0.81	1 (7%)	15,19,21	0.68	0
3	NAG	A	1078	3	14,14,15	0.60	0	15,19,21	0.73	1 (6%)
3	NAG	A	1208	1,3	14,14,15	0.42	0	15,19,21	0.73	0
3	NAG	A	1209	3	14,14,15	0.64	1 (7%)	15,19,21	0.62	0
3	NAG	B	1063	1,3	14,14,15	0.36	0	15,19,21	0.98	0
3	NAG	B	1064	3	14,14,15	0.61	0	15,19,21	0.46	0
3	NAG	E	1063	1,3	14,14,15	0.49	0	15,19,21	0.59	0
3	NAG	E	1064	3	14,14,15	0.34	0	15,19,21	0.69	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	NAG	A	1077	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1078	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1208	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	1209	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1063	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1064	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1063	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	1064	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1209	NAG	O5-C1	2.02	1.47	1.43
3	A	1077	NAG	C1-C2	2.79	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1078	NAG	C1-O5-C5	2.10	115.06	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1208	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
4	NAG	B	1077	1	14,14,15	0.44	0	15,19,21	1.01	1 (6%)
4	NAG	B	1208	1	14,14,15	0.53	0	15,19,21	0.50	0
4	NAG	E	1077	1	14,14,15	0.70	0	15,19,21	0.56	0
4	NAG	F	1077	1	14,14,15	0.76	1 (7%)	15,19,21	1.31	1 (6%)

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	NAG	B	1077	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1208	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1077	1	-	0/6/23/26	0/1/1/1
4	NAG	F	1077	1	1/1/5/7	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1077	NAG	O5-C1	-2.49	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1077	NAG	C2-N2-C7	-2.51	119.28	122.94
4	F	1077	NAG	C3-C4-C5	3.62	116.59	110.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	1077	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1077	NAG	1	0
4	B	1208	NAG	1	0
4	E	1077	NAG	1	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 ⓘ

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	457/539 (84%)	-0.24	4 (0%)	84 75	36, 85, 149, 296	0
1	B	463/539 (85%)	-0.31	7 (1%)	74 61	42, 86, 161, 250	0
1	E	462/539 (85%)	0.23	27 (5%)	24 14	72, 152, 223, 276	1 (0%)
1	F	458/539 (84%)	0.05	17 (3%)	42 27	89, 143, 196, 310	0
2	C	103/126 (81%)	0.45	16 (15%)	2 1	64, 120, 210, 233	0
2	D	104/126 (82%)	0.09	4 (3%)	41 27	64, 113, 205, 350	0
2	G	103/126 (81%)	1.23	23 (22%)	1 1	112, 173, 257, 293	0
2	H	104/126 (82%)	1.05	23 (22%)	1 1	97, 160, 240, 267	0
All	All	2254/2660 (84%)	0.07	121 (5%)	26 15	36, 125, 210, 350	1 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	83	PRO	8.9
1	A	83	PRO	8.9
2	G	70	ARG	7.6
2	G	71	GLN	6.9
2	G	127	PRO	6.9
2	G	69	ILE	6.4
1	B	83	PRO	5.7
2	H	40	CYS	5.5
2	H	137	ASN	5.5
2	G	131	GLU	5.4
1	E	46	MET	5.3
2	G	119	TYR	5.3
1	A	84	ASN	5.3
2	H	140	MET	5.0
2	G	42	LYS	4.9
2	G	51	ASN	4.8

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Mol	Chain	Res	Type	RSRZ
2	G	140	MET	4.8
2	G	50	VAL	4.7
2	C	132	GLY	4.6
2	G	132	GLY	4.5
2	D	68	ASP	4.5
2	G	40	CYS	4.5
2	H	66	ARG	4.5
1	E	83	PRO	4.4
1	F	443	HIS	4.4
2	C	133	SER	4.3
2	C	117	GLY	4.2
2	G	43	GLY	4.2
2	H	116	GLU	4.1
2	H	68	ASP	3.9
2	C	66	ARG	3.8
2	H	67	ASN	3.8
2	H	126	TYR	3.7
1	E	396	GLN	3.7
2	H	100	GLU	3.7
2	C	138	GLY	3.6
2	G	120	LEU	3.6
1	F	84	ASN	3.6
1	E	416	ASN	3.5
1	F	62	SER	3.4
2	G	49	GLU	3.3
1	E	102	LEU	3.3
2	H	45	GLU	3.3
1	F	175	THR	3.3
1	B	46	MET	3.2
2	G	115	LYS	3.2
1	E	279	GLY	3.2
1	E	101	ALA	3.2
2	H	136	ALA	3.1
2	C	116	GLU	3.1
2	H	133	SER	3.1
2	C	136	ALA	3.1
2	H	134	SER	3.1
1	E	411	ALA	3.1
1	A	162	HIS	3.0
2	D	71	GLN	3.0
1	E	401	ARG	3.0
1	E	186	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	98	LYS	2.9
1	F	33	GLY	2.9
2	H	43	GLY	2.9
2	H	132	GLY	2.9
2	G	54	LEU	2.9
2	C	140	MET	2.8
2	C	134	SER	2.8
1	E	439	ILE	2.8
2	G	128	ALA	2.8
1	F	67	PHE	2.7
1	E	84	ASN	2.7
1	E	149	HIS	2.7
1	E	423	SER	2.7
1	B	84	ASN	2.6
2	G	130	PRO	2.6
1	E	107	LYS	2.5
2	C	98	LYS	2.5
1	F	207	GLY	2.4
2	H	82	GLY	2.4
2	H	135	ALA	2.4
2	C	67	ASN	2.4
2	C	127	PRO	2.4
2	G	125	CYS	2.4
2	D	119	TYR	2.3
1	F	192	THR	2.3
1	F	485	CYS	2.3
1	F	142	SER	2.3
1	E	192	THR	2.3
1	A	439	ILE	2.3
2	C	130	PRO	2.3
2	D	70	ARG	2.3
2	C	126	TYR	2.3
1	E	422	PRO	2.3
1	E	486	GLU	2.2
1	E	338	ALA	2.2
2	H	42	LYS	2.2
1	E	234	HIS	2.2
2	H	142	CYS	2.2
2	H	47	CYS	2.2
2	G	100	GLU	2.2
1	E	93	GLU	2.2
1	F	401	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	303	HIS	2.1
1	F	61	PRO	2.1
1	F	190	ALA	2.1
2	G	41	ALA	2.1
1	B	29	VAL	2.1
1	B	160	GLY	2.1
1	B	204	TYR	2.1
2	G	133	SER	2.1
1	F	46	MET	2.1
2	H	57	SER	2.1
2	C	118	LEU	2.1
2	H	117	GLY	2.1
1	E	291	ASN	2.1
1	F	540	GLN	2.0
1	F	254	ARG	2.0
1	E	531	GLU	2.0
2	C	139	THR	2.0
1	E	208	ASN	2.0
1	E	438	PRO	2.0
1	B	485	CYS	2.0
1	E	426	LYS	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](#)

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(\AA^2)	Q<0.9
3	NAG	E	1063	14/15	0.71	0.49	4.22	191,204,213,213	0
3	NAG	E	1064	14/15	0.66	0.98	2.59	202,216,225,228	0
3	NAG	A	1077	14/15	0.80	0.49	-	141,178,197,205	0
3	NAG	B	1064	14/15	0.62	0.74	-	219,230,233,235	0
3	NAG	A	1209	14/15	0.57	0.68	-	173,191,200,201	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	1063	14/15	0.60	0.58	-	174,189,216,220	0
3	NAG	A	1078	14/15	0.71	0.65	-	188,200,224,227	0
3	NAG	A	1208	14/15	0.44	0.53	-	167,181,192,200	0

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(\AA^2)	Q<0.9
4	NAG	F	1077	14/15	0.50	0.55	-	148,163,167,172	0
4	NAG	E	1077	14/15	0.80	0.35	-	169,181,184,186	0
4	NAG	B	1077	14/15	0.81	0.35	-	109,149,161,170	0
4	NAG	B	1208	14/15	0.55	0.54	-	144,191,199,206	0

6.5 Other polymers [i](#)

There are no such residues in this entry.