



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:17 PM GMT

PDB ID : 1EWT
Title : CRYSTAL STRUCTURE OF METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1 LIGAND FREE FORM I
Authors : Kunishima, N.; Shimada, Y.; Tsuji, Y.; Jingami, H.; Morikawa, K.
Deposited on : 2000-04-27
Resolution : 3.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

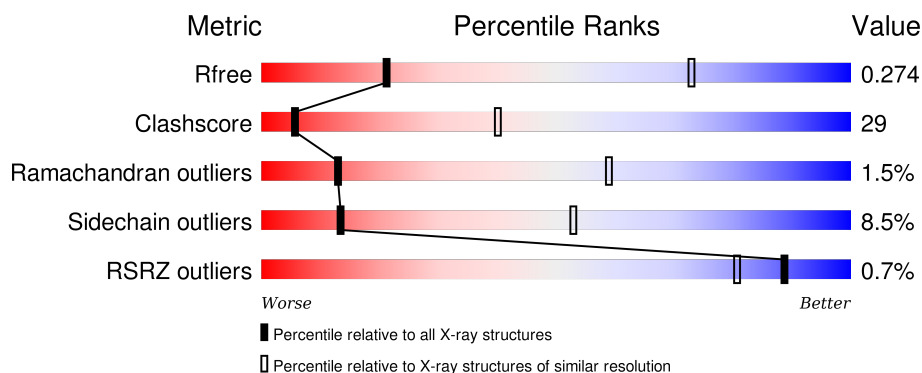
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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	490	 49% 41% 7%
1	B	490	 48% 39% 6% 7%

2 Entry composition [i](#)

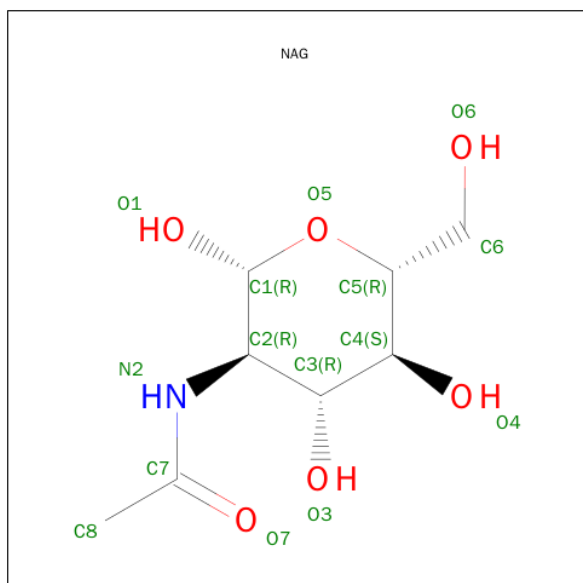
There are 3 unique types of molecules in this entry. The entry contains 7282 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	0	0
			3624	2297	632	675	20			
1	B	456	Total	C	N	O	S	0	0	0
			3624	2297	632	675	20			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

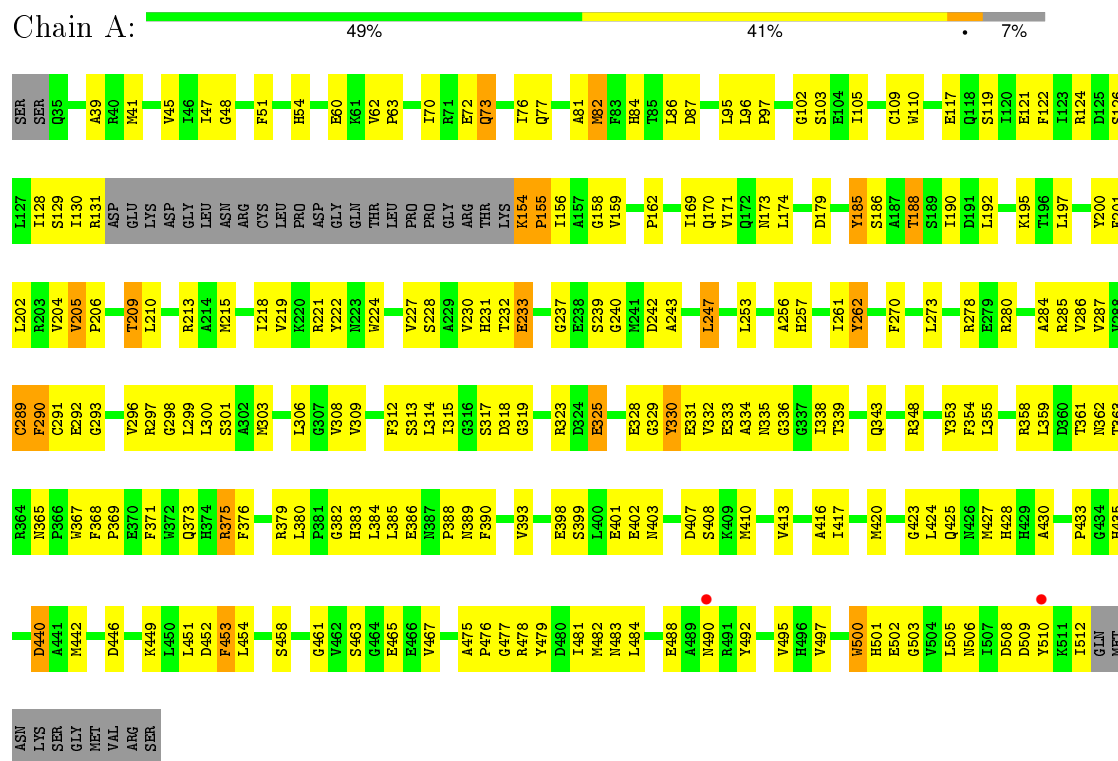


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: METABOTROPIC GLUTAMATE RECEPTOR SUBTYPE 1



SER	R448	F368	V287
	K449	P369	V288
	L450	E370	C289
	D452	F371	F290
	F453	W372	C291
SER	L454	Q373	E292
		R374	C293
		R375	V294
	S457	F376	T295
	S458	Q377	V296
	F459	R378	R297
	V460	R379	G298
	G461	L380	L299
	V462		L300
	S463	L384	S301
	G464	L385	A302
	E465	E386	N303
	V466	N387	
	V467	P388	L306
		N389	
	A475	F390	L314
	P476		
	G477	C394	
	R478		
	Y479	N397	S317
	D480	E398	D318
	I481	S399	G319
	M482	I400	N320
	N483	E401	
	L484	D407	R323
	Q485		E325
	Y486		
	T487	N410	E328
	E488		G329
	A489	V413	Y330
	N490		E331
	R491	I417	V332
	Y492	Y418	E333
	D493	A419	A334
	Y494	N420	N335
	V495	A421	G336
	H496	H422	
	V497	Q423	T339
		L424	I340
	N500	Q425	K341
	H501	H426	L342
	E502	N427	Q343
		H428	
	L505	L431	R348
	N506		
	I507	F354	Y353
	D508	H435	F354
	D509	V436	L355
	Y510		
	R511	C439	R358
	I512	D440	N362
	GLN	A441	
	MET	H442	N365
	ASN		P366
	LYS	G447	W367

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	111.44Å 111.44Å 293.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.70 12.02 – 3.71	Depositor EDS
% Data completeness (in resolution range)	99.7 (12.00-3.70) 99.8 (12.02-3.71)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 3.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.287 0.233 , 0.274	Depositor DCC
R_{free} test set	950 reflections (4.84%)	DCC
Wilson B-factor (Å ²)	92.5	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 19647 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7282	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	0.69	4/3704 (0.1%)	0.91	0/5009
1	B	0.68	4/3704 (0.1%)	0.90	0/5009
All	All	0.69	8/7408 (0.1%)	0.91	0/10018

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	224	TRP	NE1-CE2	8.77	1.49	1.37
1	B	500	TRP	NE1-CE2	8.74	1.49	1.37
1	A	500	TRP	NE1-CE2	8.70	1.48	1.37
1	A	224	TRP	NE1-CE2	8.68	1.48	1.37
1	A	110	TRP	NE1-CE2	8.59	1.48	1.37
1	A	367	TRP	NE1-CE2	8.56	1.48	1.37
1	B	110	TRP	NE1-CE2	8.55	1.48	1.37
1	B	367	TRP	NE1-CE2	7.15	1.46	1.37

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3624	0	3553	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3624	0	3552	212	0
2	B	14	0	13	1	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
All	All	7282	0	7118	419	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 29.

All (419) 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:A:362:ASN:HD21	1:A:365:ASN:HB3	1.22	1.00
1:A:278:ARG:HH11	1:A:306:LEU:HD21	1.28	0.98
1:B:278:ARG:HH11	1:B:306:LEU:HD21	1.29	0.97
1:B:407:ASP:HB3	1:B:410:MET:HB2	1.45	0.96
1:A:323:ARG:HB3	1:A:325:GLU:HG2	1.50	0.93
1:A:407:ASP:HB3	1:A:410:MET:HB2	1.49	0.93
1:B:323:ARG:HB3	1:B:325:GLU:HG2	1.50	0.91
1:A:228:SER:HB2	1:A:287:VAL:HG22	1.54	0.89
1:A:218:ILE:HD11	1:A:481:ILE:HD12	1.51	0.89
1:B:218:ILE:HD11	1:B:481:ILE:HD12	1.56	0.88
1:B:228:SER:HB2	1:B:287:VAL:HG22	1.55	0.87
1:B:461:GLY:HA3	1:B:465:GLU:HG3	1.57	0.86
1:B:257:HIS:HB2	1:B:280:ARG:HG3	1.57	0.85
1:B:300:LEU:CD2	1:B:334:ALA:HB2	2.09	0.83
1:A:162:PRO:HG3	1:A:171:VAL:HG21	1.61	0.82
1:A:39:ALA:HB3	1:A:105:ILE:HB	1.60	0.81
1:B:39:ALA:HB3	1:B:105:ILE:HB	1.62	0.81
1:A:257:HIS:HB2	1:A:280:ARG:HG3	1.62	0.80
1:B:205:VAL:HG23	1:B:206:PRO:HD2	1.61	0.80
1:A:48:GLY:O	1:A:159:VAL:HA	1.83	0.78
1:A:362:ASN:ND2	1:A:365:ASN:HB3	1.99	0.77
1:B:340:ILE:HG23	1:B:479:TYR:HB3	1.63	0.77
1:A:278:ARG:NH1	1:A:306:LEU:HD21	2.00	0.77
1:B:278:ARG:NH1	1:B:306:LEU:HD21	2.00	0.77
1:B:355:LEU:HD22	1:B:401:GLU:HG2	1.66	0.76
1:A:427:MET:HE1	1:A:449:LYS:HB3	1.65	0.76
1:A:202:LEU:HD23	1:A:202:LEU:N	2.01	0.76
1:B:368:PHE:HB3	1:B:369:PRO:HD3	1.67	0.76
1:B:475:ALA:HB1	1:B:476:PRO:HD2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:MET:CE	1:B:442:MET:HG2	2.16	0.75
1:A:300:LEU:CD2	1:A:334:ALA:HB2	2.17	0.75
1:A:382:GLY:O	1:A:386:GLU:HB2	1.86	0.75
1:A:368:PHE:HB3	1:A:369:PRO:HD3	1.68	0.74
1:B:478:ARG:HG3	1:B:478:ARG:HH11	1.52	0.74
1:B:202:LEU:HD23	1:B:202:LEU:N	2.02	0.73
1:B:323:ARG:HB3	1:B:325:GLU:CG	2.18	0.73
1:B:423:GLY:HA3	1:B:454:LEU:HD23	1.70	0.73
1:B:73:GLN:HA	1:B:77:GLN:HE21	1.53	0.73
1:A:73:GLN:HA	1:A:77:GLN:HE21	1.54	0.72
1:B:427:MET:HE1	1:B:442:MET:HG2	1.71	0.72
1:A:72:GLU:O	1:A:77:GLN:HG3	1.89	0.72
1:A:300:LEU:CD1	1:A:334:ALA:HB2	2.20	0.71
1:B:215:MET:O	1:B:219:VAL:HG23	1.91	0.71
1:A:334:ALA:O	1:A:484:LEU:HD23	1.91	0.71
1:B:358:ARG:HH11	1:B:358:ARG:HG2	1.56	0.71
1:B:205:VAL:CG2	1:B:206:PRO:HD2	2.21	0.70
1:A:230:VAL:O	1:A:289:CYS:HA	1.90	0.70
1:A:323:ARG:HB3	1:A:325:GLU:CG	2.21	0.70
1:B:89:ILE:HG21	1:B:101:LEU:HD12	1.72	0.70
1:B:300:LEU:HD22	1:B:334:ALA:HB2	1.74	0.70
1:A:355:LEU:HD22	1:A:401:GLU:HG2	1.74	0.70
1:A:227:VAL:HG12	1:A:286:VAL:HB	1.74	0.70
1:B:211:GLN:HA	1:B:479:TYR:CE1	2.28	0.69
1:A:383:HIS:CG	1:A:384:LEU:H	2.10	0.68
1:B:98:ASN:CG	2:B:601:NAG:C1	2.59	0.68
1:B:243:ALA:O	1:B:247:LEU:HB2	1.94	0.67
1:A:215:MET:O	1:A:219:VAL:HG23	1.95	0.67
1:B:213:ARG:HH11	1:B:247:LEU:HD21	1.59	0.66
1:A:243:ALA:O	1:A:247:LEU:HB2	1.95	0.66
1:A:461:GLY:HA3	1:A:465:GLU:HG3	1.76	0.66
1:A:335:ASN:OD1	1:A:336:GLY:N	2.29	0.66
1:A:446:ASP:HB3	1:A:449:LYS:HD2	1.77	0.66
1:B:227:VAL:HG12	1:B:286:VAL:HB	1.78	0.66
1:A:427:MET:HA	1:A:453:PHE:CZ	2.31	0.65
1:B:278:ARG:HH11	1:B:306:LEU:CD2	2.07	0.65
1:B:232:THR:HG21	1:B:292:GLU:OE2	1.97	0.65
1:A:461:GLY:N	1:A:465:GLU:O	2.28	0.65
1:A:202:LEU:HD23	1:A:202:LEU:H	1.62	0.64
1:A:169:ILE:HD11	1:A:192:LEU:HG	1.80	0.64
1:A:278:ARG:HH11	1:A:306:LEU:CD2	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLU:O	1:B:77:GLN:HG3	1.97	0.64
1:B:169:ILE:HD11	1:B:192:LEU:HG	1.80	0.63
1:A:95:LEU:HD12	1:A:96:LEU:N	2.13	0.63
1:B:228:SER:CB	1:B:287:VAL:HG22	2.28	0.63
1:B:202:LEU:HD23	1:B:202:LEU:H	1.62	0.63
1:B:297:ARG:HH12	1:B:328:GLU:HB3	1.62	0.63
1:A:154:LYS:NZ	1:A:154:LYS:HB2	2.12	0.63
1:B:231:HIS:HA	1:B:291:CYS:SG	2.38	0.63
1:A:402:GLU:O	1:A:403:ASN:HB2	1.99	0.63
1:A:475:ALA:HB1	1:A:476:PRO:HD2	1.79	0.63
1:A:205:VAL:HG13	1:A:206:PRO:HD2	1.80	0.63
1:A:195:LYS:NZ	1:A:201:PHE:O	2.33	0.62
1:A:297:ARG:HH12	1:A:328:GLU:HB3	1.63	0.62
1:B:343:GLN:HB2	1:B:478:ARG:O	1.99	0.62
1:B:154:LYS:NZ	1:B:154:LYS:HB2	2.14	0.62
1:A:383:HIS:ND1	1:A:384:LEU:N	2.37	0.62
1:B:300:LEU:HD21	1:B:334:ALA:HB2	1.81	0.62
1:A:232:THR:HG21	1:A:292:GLU:HB2	1.81	0.62
1:B:185:TYR:HD1	1:B:186:SER:N	1.98	0.61
1:B:477:GLY:O	1:B:478:ARG:HG2	1.99	0.61
1:B:48:GLY:O	1:B:159:VAL:HA	2.00	0.61
1:A:124:ARG:HG3	1:B:124:ARG:HH21	1.65	0.61
1:A:128:ILE:C	1:A:130:ILE:H	2.03	0.61
1:A:47:ILE:O	1:A:103:SER:HB2	2.01	0.61
1:B:47:ILE:O	1:B:103:SER:HB2	1.99	0.61
1:A:227:VAL:HG21	1:A:253:LEU:HD21	1.82	0.61
1:B:261:ILE:HD13	1:B:270:PHE:CE2	2.36	0.60
1:A:449:LYS:O	1:A:453:PHE:HB2	2.01	0.60
1:A:369:PRO:O	1:A:373:GLN:HG3	2.01	0.60
1:A:204:VAL:HG11	1:A:416:ALA:HA	1.84	0.60
1:A:232:THR:O	1:A:237:GLY:HA3	2.02	0.60
1:A:227:VAL:CG2	1:A:253:LEU:HD21	2.31	0.60
1:B:228:SER:OG	1:B:284:ALA:HB1	2.02	0.59
1:B:478:ARG:HH11	1:B:478:ARG:CG	2.15	0.59
1:B:510:TYR:CD1	1:B:510:TYR:C	2.76	0.59
1:B:425:GLN:O	1:B:428:HIS:HB3	2.03	0.59
1:B:190:ILE:HD12	1:B:208:ASP:HB2	1.85	0.59
1:B:185:TYR:CD2	1:B:413:VAL:HG22	2.38	0.58
1:A:293:GLY:HA3	1:A:323:ARG:NH1	2.19	0.58
1:A:73:GLN:NE2	1:A:73:GLN:H	2.02	0.58
1:B:325:GLU:N	1:B:325:GLU:OE1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:C	1:A:131:ARG:HG3	2.22	0.57
1:A:231:HIS:HA	1:A:291:CYS:SG	2.44	0.57
1:A:185:TYR:CD2	1:A:413:VAL:HG22	2.39	0.57
1:B:211:GLN:HE21	1:B:317:SER:HB2	1.69	0.57
1:A:261:ILE:HD13	1:A:270:PHE:CE2	2.39	0.57
1:B:369:PRO:O	1:B:373:GLN:HG3	2.05	0.57
1:A:228:SER:CB	1:A:287:VAL:HG22	2.31	0.57
1:B:213:ARG:HH11	1:B:247:LEU:CD2	2.18	0.57
1:A:124:ARG:HG3	1:B:124:ARG:NH2	2.20	0.57
1:B:227:VAL:CG2	1:B:253:LEU:HD21	2.35	0.56
1:A:158:GLY:HA3	1:A:420:MET:CE	2.35	0.56
1:A:51:PHE:HE1	1:A:185:TYR:HE2	1.53	0.56
1:B:463:SER:C	1:B:465:GLU:H	2.08	0.56
1:B:73:GLN:H	1:B:73:GLN:NE2	2.03	0.56
1:A:228:SER:OG	1:A:284:ALA:HB1	2.06	0.56
1:B:380:LEU:HD23	1:B:394:CYS:HB2	1.87	0.56
1:B:130:ILE:C	1:B:131:ARG:HG3	2.26	0.56
1:A:301:SER:HA	1:A:330:TYR:CE2	2.40	0.56
1:A:446:ASP:CB	1:A:449:LYS:HD2	2.35	0.56
1:B:335:ASN:HA	1:B:484:LEU:HD23	1.88	0.56
1:A:423:GLY:HA3	1:A:454:LEU:HD23	1.86	0.56
1:A:174:LEU:HB2	1:B:177:LEU:CD1	2.36	0.56
1:A:300:LEU:HD22	1:A:334:ALA:HB2	1.87	0.55
1:B:407:ASP:O	1:B:410:MET:HB3	2.06	0.55
1:B:323:ARG:CB	1:B:325:GLU:HG2	2.30	0.55
1:B:86:LEU:O	1:B:90:ASN:ND2	2.40	0.55
1:B:335:ASN:HD21	1:B:485:GLN:HA	1.72	0.55
1:B:331:GLU:HB3	1:B:492:TYR:CD2	2.41	0.54
1:B:478:ARG:HG3	1:B:478:ARG:NH1	2.19	0.54
1:B:463:SER:O	1:B:465:GLU:N	2.40	0.54
1:A:379:ARG:O	1:A:393:VAL:HG13	2.08	0.54
1:A:325:GLU:OE1	1:A:325:GLU:N	2.40	0.53
1:B:373:GLN:OE1	1:B:379:ARG:HA	2.08	0.53
1:A:379:ARG:HD3	1:A:390:PHE:O	2.08	0.53
1:B:451:LEU:HG	1:B:452:ASP:N	2.23	0.53
1:A:446:ASP:HB3	1:A:449:LYS:HB2	1.91	0.53
1:B:270:PHE:CE1	1:B:298:GLY:HA3	2.43	0.53
1:B:495:VAL:O	1:B:497:VAL:HG13	2.09	0.53
1:B:201:PHE:C	1:B:201:PHE:CD2	2.82	0.53
1:A:427:MET:HG2	1:A:442:MET:CE	2.39	0.53
1:B:73:GLN:HA	1:B:77:GLN:NE2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HB2	1:B:177:LEU:HD13	1.90	0.53
1:B:317:SER:O	1:B:319:GLY:N	2.41	0.53
1:B:261:ILE:HD13	1:B:270:PHE:CD2	2.43	0.53
1:A:45:VAL:HG11	1:A:424:LEU:CD1	2.39	0.53
1:B:427:MET:HE2	1:B:442:MET:HG2	1.88	0.53
1:B:119:SER:HA	1:B:122:PHE:HD2	1.74	0.52
1:B:51:PHE:HE1	1:B:185:TYR:HE2	1.55	0.52
1:A:300:LEU:HD13	1:A:334:ALA:HB2	1.90	0.52
1:B:368:PHE:HB3	1:B:369:PRO:CD	2.38	0.52
1:A:82:MET:HE2	1:A:86:LEU:HD11	1.92	0.52
1:B:335:ASN:C	1:B:335:ASN:ND2	2.62	0.52
1:A:95:LEU:HD12	1:A:96:LEU:H	1.73	0.52
1:A:232:THR:HG21	1:A:292:GLU:OE2	2.09	0.52
1:B:377:GLN:HA	1:B:390:PHE:CE2	2.44	0.52
1:B:230:VAL:O	1:B:289:CYS:HA	2.10	0.52
1:A:339:THR:OG1	1:A:482:MET:HB2	2.09	0.52
1:A:368:PHE:HB3	1:A:369:PRO:CD	2.39	0.52
1:B:340:ILE:CG2	1:B:479:TYR:HB3	2.37	0.52
1:A:270:PHE:CE1	1:A:298:GLY:HA3	2.45	0.52
1:B:301:SER:HA	1:B:330:TYR:CE2	2.45	0.52
1:B:335:ASN:ND2	1:B:485:GLN:HA	2.25	0.52
1:A:185:TYR:HD1	1:A:185:TYR:C	2.14	0.52
1:A:386:GLU:O	1:A:388:PRO:HD3	2.10	0.51
1:A:124:ARG:CG	1:B:124:ARG:NH2	2.74	0.51
1:A:185:TYR:CD1	1:A:185:TYR:C	2.84	0.51
1:B:489:ALA:C	1:B:491:ARG:H	2.12	0.51
1:A:430:ALA:HB3	1:A:453:PHE:HZ	1.75	0.51
1:A:261:ILE:HD13	1:A:270:PHE:CD2	2.46	0.51
1:B:195:LYS:HA	1:B:195:LYS:HE2	1.92	0.51
1:A:45:VAL:HG11	1:A:424:LEU:HD13	1.92	0.51
1:B:293:GLY:HA3	1:B:323:ARG:NH1	2.25	0.51
1:A:329:GLY:C	1:A:331:GLU:H	2.14	0.51
1:A:210:LEU:O	1:A:213:ARG:HB3	2.10	0.51
1:A:383:HIS:CG	1:A:384:LEU:N	2.77	0.51
1:A:73:GLN:HA	1:A:77:GLN:NE2	2.24	0.50
1:A:373:GLN:NE2	1:A:385:LEU:O	2.44	0.50
1:B:398:GLU:N	1:B:398:GLU:OE1	2.42	0.50
1:B:57:PRO:HG3	1:B:67:CYS:HA	1.93	0.50
1:A:185:TYR:HD1	1:A:186:SER:N	2.09	0.50
1:A:317:SER:O	1:A:319:GLY:N	2.44	0.50
1:B:461:GLY:N	1:B:465:GLU:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ARG:HG3	1:A:376:PHE:CE2	2.47	0.50
1:A:126:SER:O	1:A:130:ILE:HG12	2.12	0.50
1:B:505:LEU:HD12	1:B:506:ASN:N	2.26	0.50
1:A:190:ILE:HD11	1:A:239:SER:O	2.12	0.50
1:A:427:MET:CE	1:A:449:LYS:HB3	2.39	0.50
1:A:202:LEU:CD2	1:A:202:LEU:N	2.70	0.50
1:A:47:ILE:O	1:A:103:SER:HA	2.11	0.50
1:B:47:ILE:HG23	1:B:420:MET:HG2	1.94	0.50
1:B:233:GLU:HB3	1:B:262:TYR:CD2	2.47	0.49
1:A:77:GLN:O	1:A:81:ALA:N	2.43	0.49
1:A:158:GLY:HA3	1:A:420:MET:HE1	1.94	0.49
1:A:463:SER:O	1:A:465:GLU:N	2.45	0.49
1:A:119:SER:HA	1:A:122:PHE:HD2	1.75	0.49
1:A:73:GLN:HE21	1:A:73:GLN:H	1.59	0.49
1:B:227:VAL:HG21	1:B:253:LEU:HD21	1.95	0.49
1:A:483:ASN:OD1	1:A:512:ILE:HG23	2.11	0.49
1:B:77:GLN:O	1:B:81:ALA:N	2.38	0.49
1:A:124:ARG:HH21	1:B:124:ARG:HG3	1.76	0.49
1:A:505:LEU:HD12	1:A:506:ASN:N	2.28	0.49
1:B:169:ILE:HD12	1:B:192:LEU:HD21	1.95	0.49
1:B:158:GLY:HA3	1:B:420:MET:CE	2.41	0.49
1:B:62:VAL:HB	1:B:63:PRO:HD3	1.94	0.49
1:A:84:HIS:O	1:A:87:ASP:HB2	2.13	0.49
1:B:435:HIS:CD2	1:B:439:CYS:HB3	2.47	0.49
1:B:339:THR:OG1	1:B:482:MET:HB2	2.12	0.49
1:A:218:ILE:HD11	1:A:481:ILE:CD1	2.34	0.49
1:A:388:PRO:O	1:A:390:PHE:N	2.46	0.49
1:B:126:SER:O	1:B:130:ILE:HG12	2.13	0.49
1:B:122:PHE:CD1	1:B:156:ILE:HG13	2.47	0.49
1:B:45:VAL:HG11	1:B:424:LEU:CD1	2.43	0.49
1:A:306:LEU:HG	1:A:308:VAL:HG13	1.95	0.48
1:B:427:MET:HG2	1:B:431:LEU:HD12	1.95	0.48
1:B:99:ILE:HD11	1:B:428:HIS:CD2	2.48	0.48
1:A:488:GLU:CD	1:A:488:GLU:N	2.67	0.48
1:B:510:TYR:O	1:B:510:TYR:CD1	2.67	0.48
1:A:407:ASP:O	1:A:410:MET:HB3	2.13	0.48
1:A:96:LEU:N	1:A:97:PRO:HD3	2.28	0.48
1:B:478:ARG:CG	1:B:478:ARG:NH1	2.68	0.48
1:B:213:ARG:NH1	1:B:247:LEU:HD21	2.29	0.48
1:A:62:VAL:HB	1:A:63:PRO:HD3	1.96	0.48
1:A:427:MET:HE1	1:A:449:LYS:CB	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLY:HA3	1:B:420:MET:HE1	1.95	0.48
1:A:375:ARG:HG3	1:A:376:PHE:CD2	2.49	0.48
1:B:45:VAL:HG11	1:B:424:LEU:HD13	1.96	0.48
1:B:70:ILE:HD13	1:B:371:PHE:HB2	1.95	0.48
1:A:122:PHE:CD1	1:A:156:ILE:HG13	2.48	0.47
1:B:70:ILE:HD11	1:B:76:ILE:HD11	1.96	0.47
1:A:510:TYR:C	1:A:510:TYR:CD1	2.88	0.47
1:B:202:LEU:CD2	1:B:202:LEU:N	2.71	0.47
1:A:301:SER:HA	1:A:330:TYR:HE2	1.78	0.47
1:A:47:ILE:N	1:A:102:GLY:O	2.44	0.47
1:A:81:ALA:HB2	1:A:410:MET:HE1	1.95	0.47
1:B:427:MET:CG	1:B:431:LEU:HD12	2.45	0.47
1:A:190:ILE:HD13	1:A:243:ALA:HB2	1.96	0.47
1:A:47:ILE:HG23	1:A:420:MET:HG2	1.96	0.47
1:B:329:GLY:C	1:B:331:GLU:H	2.17	0.47
1:A:192:LEU:HD22	1:A:201:PHE:CD1	2.49	0.47
1:B:195:LYS:NZ	1:B:201:PHE:O	2.48	0.47
1:A:162:PRO:HG3	1:A:171:VAL:CG2	2.40	0.47
1:B:375:ARG:HG3	1:B:376:PHE:CE2	2.50	0.47
1:B:82:MET:CE	1:B:86:LEU:HD11	2.45	0.47
1:B:73:GLN:H	1:B:73:GLN:HE21	1.62	0.47
1:B:154:LYS:HB2	1:B:154:LYS:HZ2	1.79	0.46
1:B:124:ARG:O	1:B:128:ILE:HG12	2.15	0.46
1:A:121:GLU:OE2	1:A:124:ARG:NH2	2.47	0.46
1:A:232:THR:OG1	1:A:292:GLU:N	2.30	0.46
1:A:128:ILE:O	1:A:130:ILE:N	2.45	0.46
1:A:70:ILE:HD13	1:A:371:PHE:HB2	1.97	0.46
1:A:169:ILE:HD12	1:A:192:LEU:HD21	1.97	0.46
1:A:82:MET:CE	1:A:86:LEU:HD11	2.45	0.46
1:B:380:LEU:CD2	1:B:394:CYS:HB2	2.45	0.46
1:B:299:LEU:O	1:B:303:MET:HG3	2.16	0.46
1:B:190:ILE:HD11	1:B:209:THR:N	2.31	0.46
1:A:427:MET:HA	1:A:453:PHE:CE2	2.51	0.46
1:B:227:VAL:HG22	1:B:253:LEU:HD21	1.97	0.46
1:A:204:VAL:HG11	1:A:416:ALA:CA	2.44	0.46
1:A:500:TRP:CH2	1:A:503:GLY:N	2.83	0.46
1:B:362:ASN:HD21	1:B:365:ASN:HB3	1.81	0.46
1:B:211:GLN:NE2	1:B:317:SER:HB2	2.30	0.46
1:B:192:LEU:HD22	1:B:201:PHE:CD1	2.51	0.46
1:A:402:GLU:O	1:A:402:GLU:HG3	2.16	0.46
1:A:47:ILE:HD12	1:A:86:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:TYR:HB2	1:A:500:TRP:HB3	1.97	0.46
1:A:201:PHE:C	1:A:201:PHE:CD2	2.88	0.46
1:B:424:LEU:HD23	1:B:450:LEU:HD13	1.97	0.46
1:B:332:VAL:HG23	1:B:333:GLU:N	2.31	0.45
1:B:205:VAL:HG23	1:B:342:LEU:HD21	1.98	0.45
1:A:361:THR:O	1:A:363:THR:HG23	2.15	0.45
1:B:454:LEU:O	1:B:457:SER:HB2	2.15	0.45
1:A:335:ASN:ND2	1:A:492:TYR:CE1	2.84	0.45
1:B:98:ASN:HB2	1:B:436:VAL:HG12	1.97	0.45
1:A:154:LYS:HZ2	1:A:154:LYS:HB2	1.78	0.45
1:B:185:TYR:CE2	1:B:413:VAL:HG22	2.52	0.45
1:B:317:SER:C	1:B:319:GLY:H	2.20	0.45
1:B:270:PHE:O	1:B:273:LEU:HB3	2.17	0.45
1:A:188:THR:HG22	1:A:206:PRO:O	2.17	0.45
1:A:296:VAL:O	1:A:299:LEU:N	2.50	0.45
1:A:239:SER:OG	1:A:240:GLY:N	2.49	0.45
1:A:461:GLY:HA3	1:A:465:GLU:CG	2.45	0.45
1:A:128:ILE:C	1:A:130:ILE:N	2.71	0.45
1:B:508:ASP:OD1	1:B:510:TYR:CD2	2.70	0.45
1:A:495:VAL:O	1:A:497:VAL:HG13	2.16	0.45
1:B:84:HIS:O	1:B:87:ASP:HB2	2.16	0.45
1:A:458:SER:HA	1:A:467:VAL:O	2.16	0.45
1:B:301:SER:HA	1:B:330:TYR:HE2	1.82	0.44
1:A:70:ILE:HD11	1:A:76:ILE:HD11	1.99	0.44
1:A:343:GLN:HE21	1:A:343:GLN:HB2	1.47	0.44
1:B:332:VAL:HG23	1:B:333:GLU:H	1.82	0.44
1:B:483:ASN:OD1	1:B:512:ILE:HG23	2.17	0.44
1:A:463:SER:C	1:A:465:GLU:H	2.21	0.44
1:A:317:SER:C	1:A:319:GLY:H	2.21	0.44
1:A:82:MET:HA	1:A:417:ILE:CD1	2.47	0.44
1:A:425:GLN:O	1:A:428:HIS:HB3	2.16	0.44
1:B:190:ILE:CD1	1:B:208:ASP:HB2	2.46	0.44
1:A:501:HIS:C	1:A:502:GLU:HG2	2.38	0.44
1:A:130:ILE:O	1:A:130:ILE:HG22	2.17	0.44
1:A:343:GLN:NE2	1:A:478:ARG:HB3	2.31	0.44
1:A:359:LEU:HD11	1:A:369:PRO:HA	2.00	0.44
1:A:205:VAL:HG13	1:A:206:PRO:CD	2.45	0.44
1:B:320:TRP:O	1:B:323:ARG:HG3	2.18	0.44
1:B:358:ARG:HH11	1:B:358:ARG:CG	2.28	0.44
1:A:124:ARG:O	1:A:128:ILE:HG12	2.17	0.44
1:A:204:VAL:CG1	1:A:416:ALA:HA	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:VAL:HB	1:A:314:LEU:HD23	1.99	0.43
1:B:341:LYS:HG2	1:B:342:LEU:N	2.33	0.43
1:A:190:ILE:CG2	1:A:209:THR:H	2.30	0.43
1:A:124:ARG:CG	1:B:124:ARG:HH21	2.31	0.43
1:A:490:ASN:O	1:A:490:ASN:CG	2.55	0.43
1:A:300:LEU:HD21	1:A:334:ALA:HB2	1.95	0.43
1:B:130:ILE:HG22	1:B:130:ILE:O	2.18	0.43
1:B:211:GLN:NE2	1:B:318:ASP:OD1	2.49	0.43
1:B:82:MET:HE2	1:B:86:LEU:HD11	2.01	0.43
1:B:236:TYR:CE2	1:B:290:PHE:CD2	3.06	0.43
1:B:218:ILE:HD11	1:B:481:ILE:HG23	2.00	0.43
1:A:195:LYS:HE2	1:A:195:LYS:HA	2.01	0.43
1:B:55:HIS:ND1	1:B:71:ARG:HD2	2.33	0.43
1:A:154:LYS:HG2	1:A:155:PRO:HD2	2.00	0.43
1:A:73:GLN:HB2	1:A:73:GLN:HE21	1.54	0.43
1:A:373:GLN:OE1	1:A:380:LEU:HG	2.18	0.43
1:B:82:MET:HA	1:B:417:ILE:CD1	2.49	0.43
1:A:84:HIS:HB2	1:A:353:TYR:CE2	2.54	0.43
1:B:449:LYS:O	1:B:453:PHE:HB2	2.19	0.43
1:B:205:VAL:CG2	1:B:342:LEU:HD21	2.48	0.43
1:A:54:HIS:O	1:A:109:CYS:HA	2.19	0.43
1:A:398:GLU:OE1	1:A:398:GLU:N	2.38	0.43
1:A:169:ILE:HG22	1:A:170:GLN:N	2.33	0.43
1:A:185:TYR:CE2	1:A:413:VAL:HG22	2.53	0.43
1:B:501:HIS:C	1:B:502:GLU:HG2	2.38	0.43
1:A:124:ARG:NH2	1:B:124:ARG:HG3	2.33	0.42
1:B:380:LEU:O	1:B:386:GLU:HG3	2.19	0.42
1:A:233:GLU:HB3	1:A:262:TYR:CE2	2.54	0.42
1:A:451:LEU:HG	1:A:452:ASP:N	2.33	0.42
1:A:47:ILE:O	1:A:103:SER:CB	2.66	0.42
1:B:331:GLU:HG2	1:B:492:TYR:HB2	2.02	0.42
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.83	0.42
1:A:221:ARG:C	1:A:222:TYR:HD2	2.22	0.42
1:B:221:ARG:HB2	1:B:221:ARG:HE	1.64	0.42
1:B:185:TYR:O	1:B:205:VAL:HG11	2.19	0.42
1:A:240:GLY:HA3	1:A:290:PHE:CE1	2.54	0.42
1:B:47:ILE:HD12	1:B:86:LEU:HD21	2.01	0.42
1:B:122:PHE:HD1	1:B:156:ILE:HG13	1.84	0.42
1:A:262:TYR:HA	1:A:262:TYR:HD2	1.74	0.42
1:B:221:ARG:C	1:B:222:TYR:HD2	2.22	0.42
1:A:306:LEU:HG	1:A:306:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:O	1:A:330:TYR:HD1	2.02	0.42
1:A:270:PHE:O	1:A:273:LEU:HB3	2.20	0.42
1:B:241:MET:HG3	1:B:245:LYS:HG3	2.00	0.42
1:B:185:TYR:CD1	1:B:186:SER:N	2.83	0.42
1:B:47:ILE:N	1:B:102:GLY:O	2.49	0.42
1:A:358:ARG:HG2	1:A:358:ARG:NH1	2.34	0.42
1:A:423:GLY:HA3	1:A:454:LEU:CD2	2.48	0.42
1:B:477:GLY:C	1:B:478:ARG:HG2	2.40	0.42
1:B:84:HIS:HB2	1:B:353:TYR:CE2	2.55	0.42
1:A:354:PHE:O	1:A:354:PHE:CG	2.72	0.42
1:B:358:ARG:NH1	1:B:358:ARG:HG2	2.30	0.42
1:B:192:LEU:HD22	1:B:201:PHE:CG	2.54	0.42
1:A:173:ASN:HA	1:A:173:ASN:HD22	1.74	0.42
1:A:308:VAL:O	1:A:309:VAL:CG2	2.68	0.42
1:A:119:SER:O	1:A:122:PHE:HB2	2.20	0.42
1:A:463:SER:C	1:A:465:GLU:N	2.73	0.41
1:B:328:GLU:O	1:B:330:TYR:HD1	2.02	0.41
1:A:124:ARG:NH2	1:B:124:ARG:CG	2.83	0.41
1:B:47:ILE:O	1:B:103:SER:HA	2.19	0.41
1:A:500:TRP:CZ3	1:A:502:GLU:HA	2.55	0.41
1:B:335:ASN:ND2	1:B:336:GLY:N	2.68	0.41
1:B:387:ASN:OD1	1:B:389:ASN:N	2.50	0.41
1:B:343:GLN:HG3	1:B:480:ASP:CG	2.41	0.41
1:B:232:THR:O	1:B:237:GLY:HA3	2.20	0.41
1:A:407:ASP:CB	1:A:410:MET:HB2	2.35	0.41
1:B:287:VAL:HB	1:B:314:LEU:HD23	2.02	0.41
1:B:379:ARG:HB3	1:B:387:ASN:O	2.20	0.41
1:A:368:PHE:CB	1:A:369:PRO:HD3	2.45	0.41
1:B:331:GLU:O	1:B:335:ASN:HB2	2.20	0.41
1:A:117:GLU:HG3	1:B:127:LEU:HD13	2.03	0.41
1:A:335:ASN:ND2	1:A:492:TYR:HE1	2.17	0.41
1:B:188:THR:HG22	1:B:206:PRO:O	2.20	0.41
1:A:206:PRO:HB3	1:A:477:GLY:HA2	2.03	0.41
1:B:154:LYS:HG2	1:B:155:PRO:HD2	2.03	0.41
1:B:296:VAL:O	1:B:299:LEU:N	2.52	0.41
1:B:459:PHE:CZ	1:B:467:VAL:HG11	2.55	0.41
1:A:84:HIS:HB2	1:A:353:TYR:CD2	2.56	0.41
1:B:435:HIS:CD2	1:B:439:CYS:CB	3.04	0.41
1:B:214:ALA:HA	1:B:500:TRP:NE1	2.35	0.41
1:B:188:THR:HA	1:B:203:ARG:NH1	2.36	0.41
1:B:343:GLN:HG3	1:B:480:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:CD1	1:A:192:LEU:HG	2.51	0.41
1:B:384:LEU:HG	1:B:384:LEU:H	1.66	0.41
1:A:407:ASP:OD2	1:A:408:SER:N	2.54	0.41
1:B:208:ASP:O	1:B:211:GLN:HB2	2.20	0.41
1:B:169:ILE:CD1	1:B:192:LEU:HG	2.50	0.40
1:B:418:TYR:O	1:B:421:ALA:HB3	2.21	0.40
1:B:56:GLN:HA	1:B:57:PRO:HD3	1.95	0.40
1:A:323:ARG:CB	1:A:325:GLU:HG2	2.35	0.40
1:B:317:SER:C	1:B:319:GLY:N	2.75	0.40
1:A:192:LEU:HD22	1:A:201:PHE:CG	2.56	0.40
1:B:489:ALA:C	1:B:491:ARG:N	2.75	0.40
1:B:236:TYR:CZ	1:B:290:PHE:HE2	2.40	0.40
1:B:222:TYR:CD2	1:B:222:TYR:N	2.87	0.40
1:B:222:TYR:HD1	1:B:224:TRP:CH2	2.38	0.40
1:A:179:ASP:HA	1:A:200:TYR:CE2	2.56	0.40
1:A:315:ILE:HA	1:A:338:ILE:O	2.21	0.40
1:A:303:MET:CE	1:A:312:PHE:HD2	2.34	0.40
1:A:433:PRO:C	1:A:435:HIS:H	2.24	0.40
1:A:309:VAL:HG11	1:A:332:VAL:HG12	2.03	0.40
1:A:355:LEU:HD22	1:A:401:GLU:CG	2.49	0.40
1:B:236:TYR:CE2	1:B:290:PHE:CE2	3.10	0.40

There are no symmetry-related clashes.

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	452/490 (92%)	391 (86%)	55 (12%)	6 (1%)	15	62
1	B	452/490 (92%)	397 (88%)	47 (10%)	8 (2%)	11	56
All	All	904/980 (92%)	788 (87%)	102 (11%)	14 (2%)	13	59

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ALA
1	A	389	ASN
1	B	256	ALA
1	A	318	ASP
1	A	330	TYR
1	A	440	ASP
1	B	318	ASP
1	B	440	ASP
1	B	508	ASP
1	A	129	SER
1	B	490	ASN
1	B	502	GLU
1	B	330	TYR
1	B	447	GLY

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	392/422 (93%)	365 (93%)	27 (7%)	19	61
1	B	392/422 (93%)	352 (90%)	40 (10%)	9	43
All	All	784/844 (93%)	717 (92%)	67 (8%)	13	53

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	60	GLU
1	A	73	GLN
1	A	82	MET
1	A	154	LYS
1	A	155	PRO
1	A	185	TYR
1	A	188	THR
1	A	197	LEU

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Mol	Chain	Res	Type
1	A	205	VAL
1	A	209	THR
1	A	233	GLU
1	A	242	ASP
1	A	247	LEU
1	A	262	TYR
1	A	289	CYS
1	A	290	PHE
1	A	313	SER
1	A	325	GLU
1	A	333	GLU
1	A	348	ARG
1	A	375	ARG
1	A	399	SER
1	A	440	ASP
1	A	453	PHE
1	A	508	ASP
1	A	509	ASP
1	B	37	SER
1	B	41	MET
1	B	60	GLU
1	B	73	GLN
1	B	82	MET
1	B	95	LEU
1	B	126	SER
1	B	129	SER
1	B	154	LYS
1	B	155	PRO
1	B	185	TYR
1	B	188	THR
1	B	190	ILE
1	B	197	LEU
1	B	202	LEU
1	B	204	VAL
1	B	210	LEU
1	B	211	GLN
1	B	242	ASP
1	B	247	LEU
1	B	262	TYR
1	B	289	CYS
1	B	290	PHE
1	B	294	MET

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Mol	Chain	Res	Type
1	B	325	GLU
1	B	335	ASN
1	B	343	GLN
1	B	348	ARG
1	B	375	ARG
1	B	379	ARG
1	B	384	LEU
1	B	397	ASN
1	B	399	SER
1	B	440	ASP
1	B	452	ASP
1	B	453	PHE
1	B	487	THR
1	B	493	ASP
1	B	509	ASP
1	B	510	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	77	GLN
1	A	173	ASN
1	A	176	GLN
1	A	250	GLN
1	A	343	GLN
1	A	362	ASN
1	B	73	GLN
1	B	77	GLN
1	B	173	ASN
1	B	176	GLN
1	B	211	GLN
1	B	250	GLN
1	B	335	ASN
1	B	343	GLN
1	B	362	ASN
1	B	435	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
3	SO4	A	701	-	4,4,4	0.27	0	6,6,6	0.22	0
3	SO4	A	702	-	4,4,4	0.21	0	6,6,6	0.26	0
2	NAG	B	601	1	14,14,15	0.84	0	15,19,21	0.88	1 (6%)
3	SO4	B	703	-	4,4,4	0.24	0	6,6,6	0.13	0
3	SO4	B	704	-	4,4,4	0.22	0	6,6,6	0.12	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	SO4	A	701	-	-	0/0/0/0	0/0/0/0
3	SO4	A	702	-	-	0/0/0/0	0/0/0/0
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
3	SO4	B	703	-	-	0/0/0/0	0/0/0/0
3	SO4	B	704	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	601	NAG	C2-N2-C7	-2.10	120.34	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	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 [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	456/490 (93%)	-0.43	2 (0%) 93 88	32, 69, 110, 123	0
1	B	456/490 (93%)	-0.42	4 (0%) 85 75	31, 68, 112, 124	0
All	All	912/980 (93%)	-0.42	6 (0%) 89 81	31, 69, 112, 124	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	ASN	3.3
1	A	490	ASN	3.2
1	B	223	ASN	2.7
1	B	35	GLN	2.4
1	B	389	ASN	2.3
1	A	510	TYR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	B	703	5/5	0.94	0.20	-0.13	88,89,89,90	0
3	SO4	B	704	5/5	0.89	0.22	-0.75	92,92,93,93	0
3	SO4	A	701	5/5	0.92	0.17	-0.88	81,82,83,83	0
3	SO4	A	702	5/5	0.98	0.18	-0.94	72,73,74,74	0
2	NAG	B	601	14/15	0.73	0.41	-	93,96,100,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.